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TITLE CHEMISTRY CALCULATIONS RELATING TO AIM

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Chemistry Calculations Relating to AIM

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Abstract

This paper describes some single-cell RF-heating and air chemistry computations that are intended to model the conditions of an AIM experiment, either in a laboratory environment or in the atmosphere. For a pulsed mode of RF-induced ionization using repetitive 120-ns pulses with 1-ns separation we examine the relative amounts of power required to sustain ionization in the second and subsequent pulses compared to the first pulse. We also compare power requirements for sustained ionization at a pressure of 1 Torr (46 km altitude) and at 0.03 Torr (74 km altitude). The power needed in the 0.03-Torr case is substantially less than in the higher-pressure case. We find that at both pressures, using the RF power densities required to sustain ionization the neutral gas is heated very rapidly to temperatures exceeding 5000 K, leading to strong turbulence. We follow the chemical evolution of 55 species of atoms, molecules and ions, and we pay particular attention to the rate of production of N and NO, because of the effects of those species on the concentrations of stratospheric ozone. The N and NO production rates are not sufficient to cause serious concerns about ozone depletion. In the case representing 74 km altitude ($P = 0.03$ Torr) we find that quite high concentrations of NO will exist in the vicinity of the artificial ionization patch, leading to the possibility of enhanced local D-region ionization caused by the ionization of NO by solar Lyman-alpha.

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1 Introduction

This paper describes some single-cell air chemistry and RF-heating computations that are intended to approximate the conditions of an AIM experiment, either in a laboratory environment or in the atmosphere. Some questions to be addressed are:

1. How much RF power is absorbed by the air?
2. How rapidly does the temperature rise?
3. What changes in chemical composition are produced in the affected air?
4. How do these chemistry results relate to possible environmental effects of a full-scale AIM facility? In particular, will significant quantities of nitrogen oxides be added to the upper atmosphere?

We have done the computations in three stages. The first stage is done with a model of the propagation/absorption/reflection of high power RF waves in air including the self-consistent treatment of electron heating, collisional excitation and ionization of the air, and electron attachment and recombination, and including both time- and spatial variations of all quantities in the direction of propagation of the RF waves. Because of computer costs this model only treats a single RF pulse and a brief post-pulse period extending to about 10^{-6} seconds.

The second stage of the calculation treats the detailed chemistry at one location, using the previously-computed electron temperature vs time as input, together with the initial electron density. It includes the time evolution of concentrations of 55 chemical species and of the neutral temperature, and it is sufficiently fast-running that it can treat a sequence of 20 or more pulses. It is typically found that at the start of the second and later pulses the residual electron density is much higher than it was before the start of the first pulse. Therefore, a lower RF power density (or lower electron temperature) is required in the second pulse to raise the electron density to the same peak value as that attained in the first. Since the peak electron density reached in the first pulse is essentially that required to reflect the RF wave, larger electron densities than that are physically unreasonable in the AIM scenario. Therefore, for pulses after the first, in order to obtain the same peak electron density, we must reduce the input electron temperatures (equivalent to reducing the RF power levels). We arbitrarily multiply the input first-pulse electron temperatures by a factor

(≤ 1), which is determined by trial and error to be such as to produce the desired limiting electron density. With the factor correctly adjusted the electron density-vs-time plot exhibits a regular sawtooth shape. On the other hand the plots of N, NO and O concentrations and that of the neutral temperature resemble the *time-integral* of the electron-ion production rate. It is found that the air composition and temperature are substantially altered within 20 pulses (20 milliseconds).

Because of the requirement of the chemistry model to use small time steps to resolve the leading edge of each pulse in detail it takes a significant amount of computer time to follow 20 pulses. It is too expensive to use to simulate a long-running AIM experiment lasting several seconds, minutes or hours. Therefore we developed a third-stage chemistry model. The third-stage model is similar to the second-stage model just described except that it approximates the effects of a sequence of many RF pulses by substituting a steady input ionization source whose strength is chosen such as to produce approximately the same electron, N, NO and O densities at times of 10 to 20 ms as does the second-stage model. This model is fast-running and can be used to simulate AIM experiments of any reasonable duration. However, the computations show typically that the neutral gas temperature rises beyond 5000 K in less than a second, at which time thermal ionization processes begin to be faster than the ionization produced by the RF wave directly. At this point we choose to stop.

The second- and third-stage models do not include any spatial dependencies - i.e. they represent a closed system. They allow us to compute the concentrations of chemical species such as N, NO, O, O_3 , etc. within the local region excited by the RF beam but not the rate of emission of these species into the rest of the atmosphere. To do a detailed computation of the amounts of NO_x , etc. released to the environment would require a 2-D multi-cell diffusion, transport and chemistry model of a sort that we have not built. However, it is clear that the local atmospheric mixing would be dominated by locally-driven turbulence (since we have found that the local temperatures exceed 5000 K), and it is unlikely that we could find a reliable algorithm to describe this turbulence. Because of this problem the construction of the 2-D diffusion model does not seem worthwhile. On the other hand we can make some simple hand-calculated estimates of the NO_x release rate based on the third-stage model results. The

results will be described.

2 Specific Computations

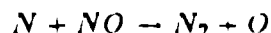
2.1 Case I: $P = 1$ Torr

In one scenario the RF beam geometry is supposed to be such that the ionization patch would be formed at about 46 km altitude, where $P \approx 1$ Torr.

Figure 1 shows the phase-one computation of the electron density vs time and electron temperature vs time during and shortly after the first pulse at a location near the center of the patch. Both n_e and T_e rise rapidly during the pulse and then decay slowly.

Figure 2a,b shows the input T_e and computed n_e from a phase 2 computation representing a train of 20 pulses. During the first pulse the input T_e vs t was taken to be identical to that computed in phase 1 (Fig. 1b). For subsequent pulses the first-pulse $T_e(t)$ was multiplied by the factor 0.53, determined by trial-and-error, so as to produce the same peak electron density as that computed for the first pulse. The time evolutions of the T_e and n_e during the 120-ns-long RF pulses are not resolved in the figure, which shows only a sequence of discontinuous electron density increases followed by a sequence of decays due to dissociative ion-electron recombination.

The pressure was held constant at 1 Torr - i.e. by the inclusion of a volume rate of change term in each of the chemical rate equations. Figure 3a shows the computed neutral temperature $T_n(t)$, which is based on the amounts of energy input in each RF pulse and assumes a constant specific heat $C_p = \frac{5}{2}k$ erg/deg·molecule (where k is Boltzmann's constant). Figures 3b, 4a and 4b show the corresponding computed concentrations of N, NO and O. Those three species are closely coupled through the chemical reaction



During the brief 20-ns duration of this simulation the temperature rise is not sufficient to affect the chemical rate coefficients very strongly, so the evolution of the chemical concentrations seems fairly simple and regular.

To continue the computation to longer times we switch to the phase-3 approximation which replaces the sequence of RF pulses (electron temperature excursions) by a quasi-steady ionization source. The latter is specified as $Q = \alpha_{eff} n_{e(max)}^2$ ion-pairs/cm³ · s, where $n_{e(max)}$ is an electron density level chosen to match the results of the phase 2 computation and α_{eff} is an effective ion-electron recombination rate coefficient, computed interactively as the weighted average of the recombination coefficients of the various positive ion species present. The electron and neutral temperatures are assumed to be equal.

Some of the phase-3 computed results are shown in Figs. 5a,b and 6a,b,c. Figure 5a,b shows the electron density and the temperature. The temperature reached 5000 K in 1.5 seconds, at which point the calculation was stopped. The electron density rises very rapidly to a plateau and remains constant thereafter at a value close to the average value of n_e that was computed in phase 2. The computed N, NO and O concentrations are plotted in Figs. 6a,b,c. At early times they are close to the values computed at similar times with the phase-2 model. At later times the N and NO concentrations exhibit some complicated undulations, but the O concentration increases steadily. At 1.5 seconds, the end of the run, O₂ is mostly dissociated into atoms, and the heated region has expanded to about 15 times its original volume. The final NO concentration at 1.5 s is close to 10¹⁴ cm⁻³, and it is about three times larger than the N concentration.

One of the purposes of this study was to examine possible environmental problems that could arise from a full-scale AIM operation. One concern is the rate at which nitrogen oxides would be added to the upper atmosphere, because of the well known effects of stratospheric NO_x concentrations on the ozone balance. It would have to be shown that the rate of increased NO_x injection would not be sufficient to affect the global or regional NO_x concentrations.

As we have noted, this model thus far represents a closed system. The computations show that very large concentrations of NO_x are produced locally, but they do not address the question of the rates of addition of NO_x to the rest of the atmosphere. However, we can address the latter problem in an approximate way as follows.

We found that the RF heating led to a temperature rise rate of about 3000 degK/s. Such a heating rate would certainly lead to intense turbulence and rapid mixing, so that N, NO, and other chemical products would be injected into the surrounding atmosphere. We also

found that on a time scale of 1 to 1.5 s the average rate of NO production per unit volume was about $6 \times 10^{13} \text{ cm}^{-3} \text{ s}^{-1}$. If we assume that the heated region is 10 cm in depth and extends over a square kilometer, then the volume is 10^{11} cm^3 and the rate of NO_x production and injection into the atmosphere is about 6×10^{24} molecules/s. The total inventory of NO_x in the global stratosphere is about 10^{34} molecules. Therefore the RF heating activity would be capable of doubling the global NO_x inventory in about 1.5×10^9 seconds, or about 50 years. This rate does not seem alarming.

On the other hand, on a regional scale the NO_x injection problems could be more severe. The normal NO_x inventory over an area of 1000 by 1000 square kilometers is about 10^{31} molecules. If we take the injection rate due to the AIM to be $6 \times 10^{24} \text{ s}^{-1}$ then the NO_x doubling time comes out to be about 20 days. This time is substantially longer than the atmospheric changeover time for a 1000 by 1000 km^2 region (about 2 days), and we can conclude that an AIM operation running continuously would not produce a noticeable increase in regional NO_x concentrations.

It is possible that there would be a faintly-visible brown NO_2 cloud in the near vicinity of the heated region.

Assuming perfect efficiency (i.e. no reflection of the RF waves) and an ionized volume of 10^{11} cm^3 to obtain sustained ionization would require an average RF power of 120 Megawatts. Taking the duty factor to be 1.2×10^{-4} this implies a peak power of 10^6 Megawatts per pulse after the first pulse.

2.2 Case II: $P = 0.03$ Torr

We ran a similar set of calculations for the lower pressure of 0.03 Torr, representing an altitude of about 74 km. Figure 8a,b shows the results of the phase-1 computation of electron density vs time and electron temperature vs time during and shortly after the first pulse.

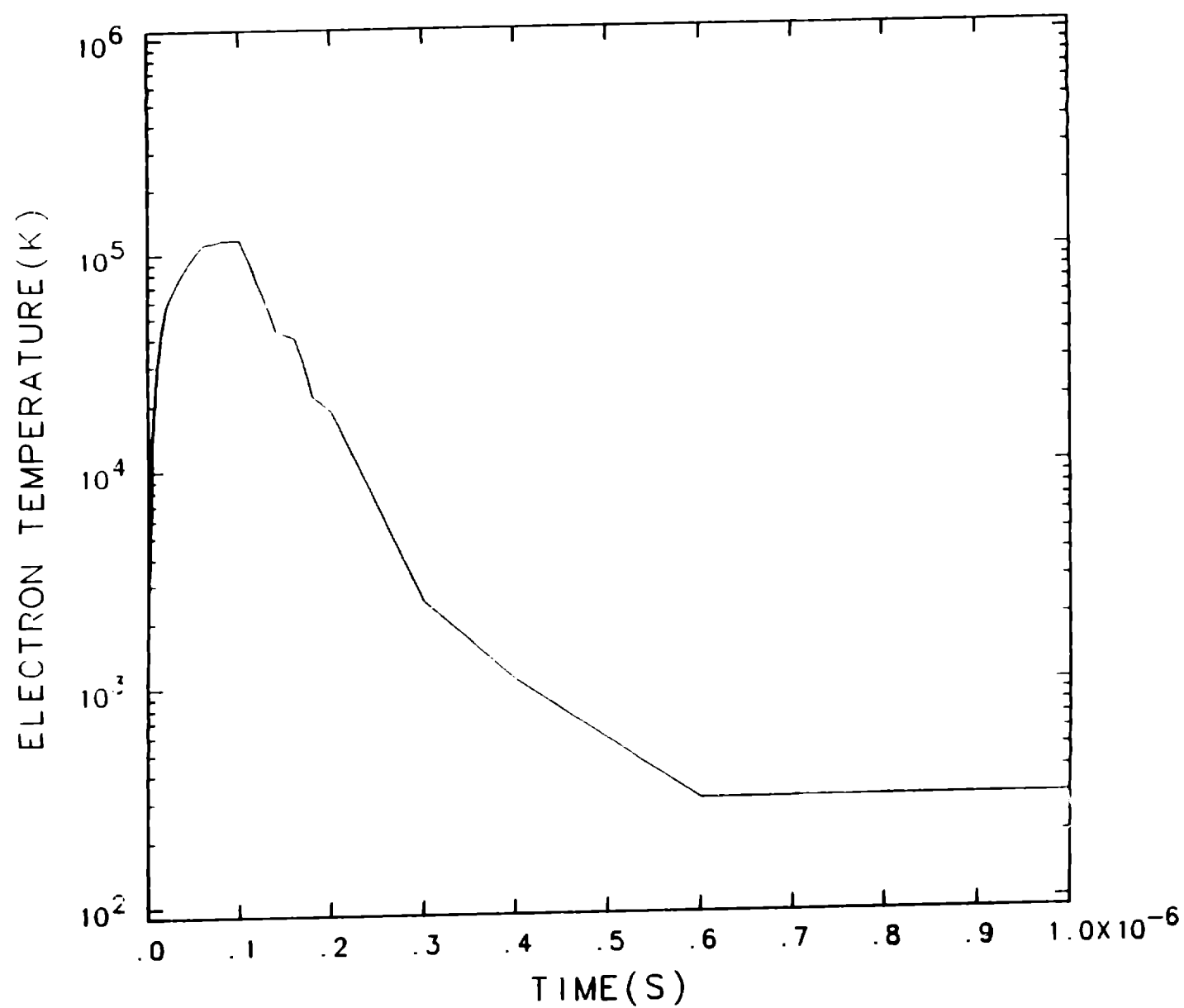
Figures 9a,b, 10a,b and 11a,b show results of a phase-2 computation for 20 pulses. It was found that to obtain the same peak electron density in the second and subsequent pulses as that obtained in the first pulse the electron temperatures had to be scaled down by the factor 0.03. The plots of $n_e(t)$ and $T_e(t)$ are shown in Figs. 9a,b. The plots of the neutral temperature and the concentrations of N, NO and O are shown in Figs. 10a,b and 11a,b. Because of the smaller ratio

of peak electron density to neutral molecular density in this case the neutral temperature rises faster than in the 1-Torr case. Results of the phase-3 computation are shown in Figs. 12a,b and 13a,b,c. 14a,b. The neutral temperature reached 5000 K in 0.75 s, at which point the calculation was stopped. At that point the heated air had expanded by a factor of about 15 and O_2 was mostly dissociated into atoms. The peak NO concentration was about 1.2×10^{12} and the N atom concentration was about a factor of two smaller.

On the question of injection of NO_x it is clear that in this case the rate of increase of NO_x concentrations relative to the total global or regional inventory is smaller than in the 1-Torr case. Therefore the effect on stratospheric ozone should be totally negligible. However the local increase of NO and N concentrations in the near vicinity of the heated region would be very large. The local concentration of artificially-produced NO, of order $10^{12} cm^{-3}$, would be about 5.5 orders of magnitude larger than the ambient NO concentration. The increase in atomic N concentrations would be about 10^7 above background. Since NO is ionizable by solar H-Ly- α radiation this could result in a considerable enhancement of ionization outside of the region of direct RF-induced ionization. The effects of this diffuse enhanced D-region ionization remain to be investigated.

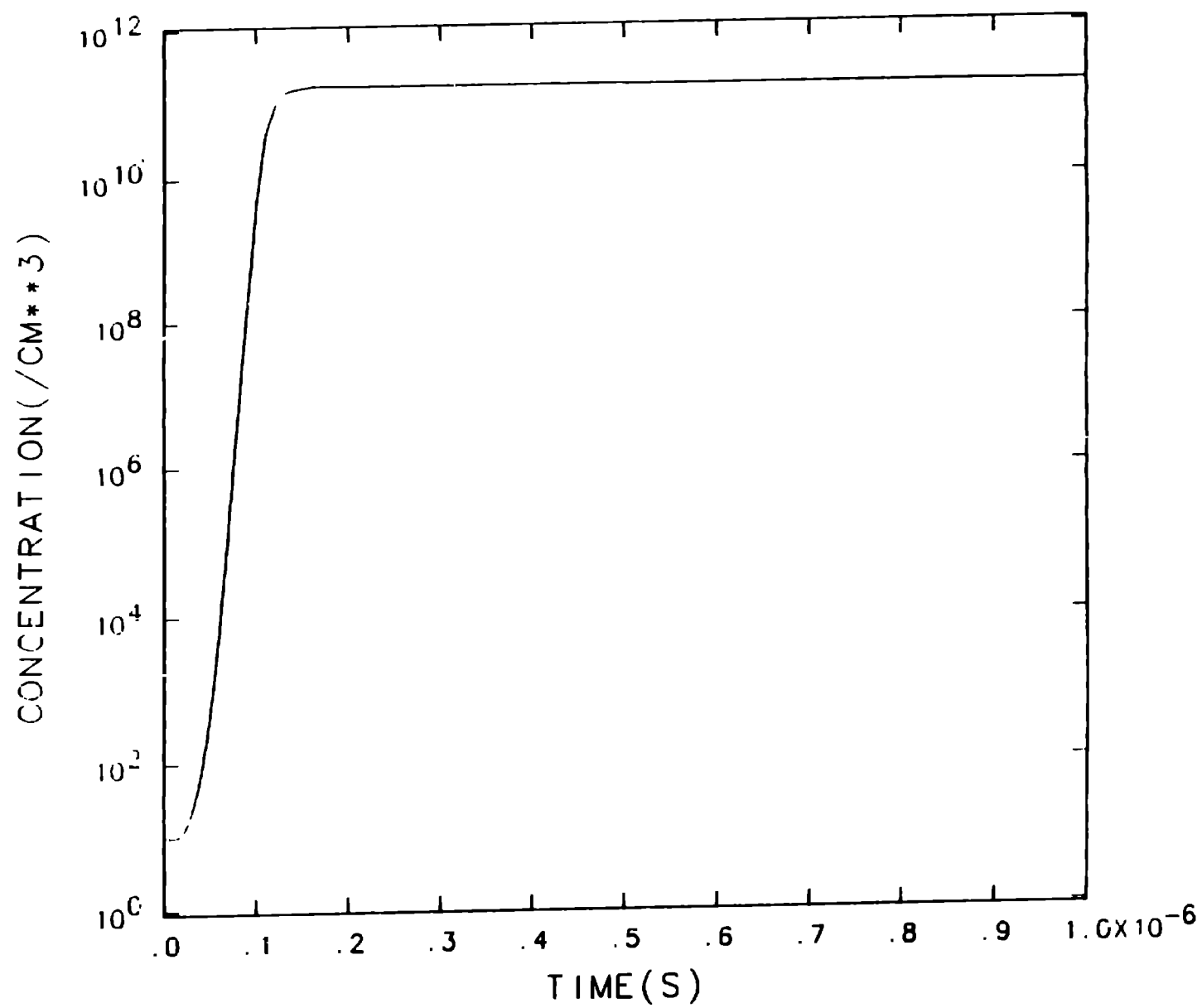
The RF power requirement for maintaining the ionization patch at this pressure (altitude) is about 10 times smaller than in the 1-Torr case.

PRESSURE 1.00



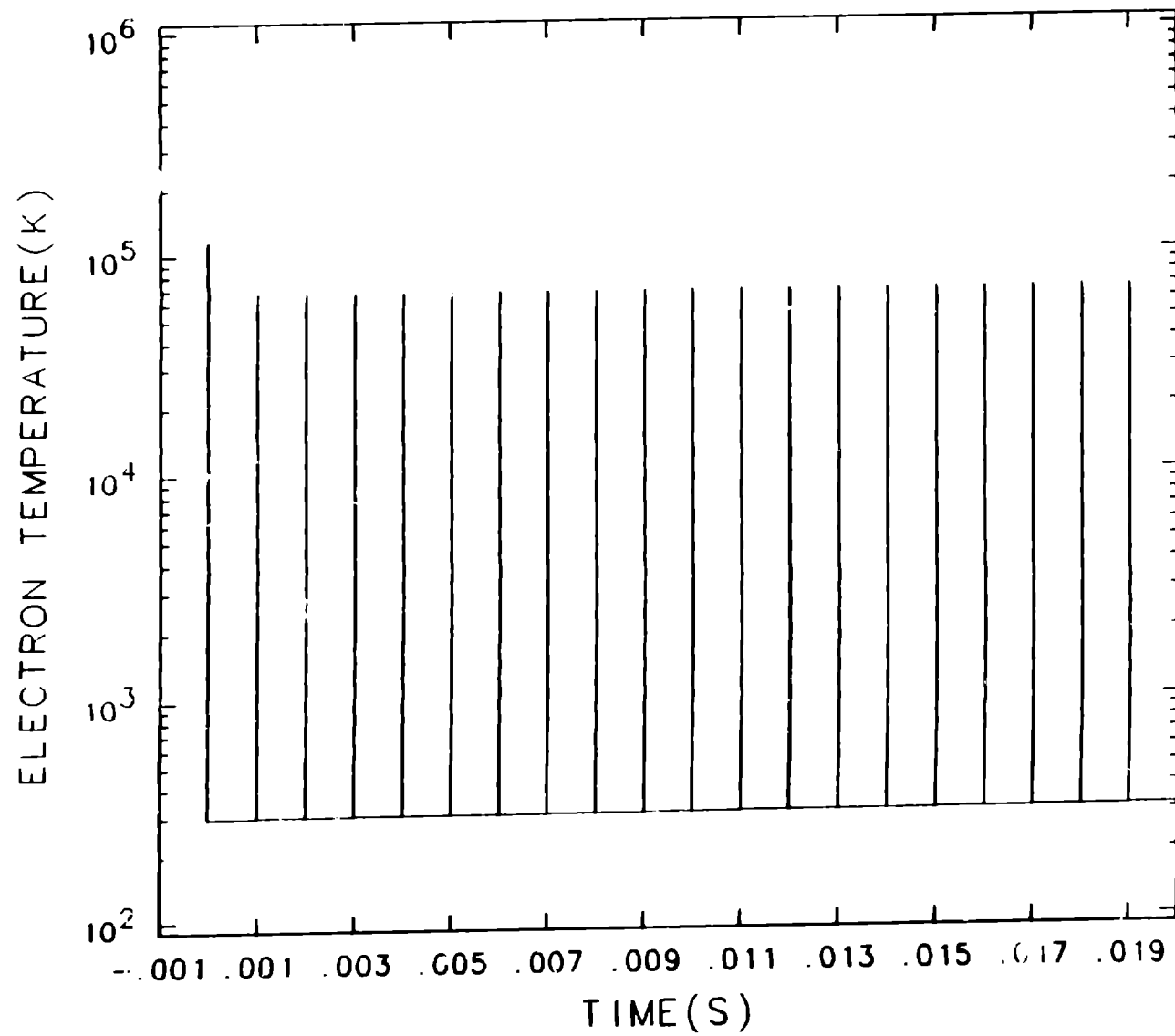
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E PRESSURE 1.00



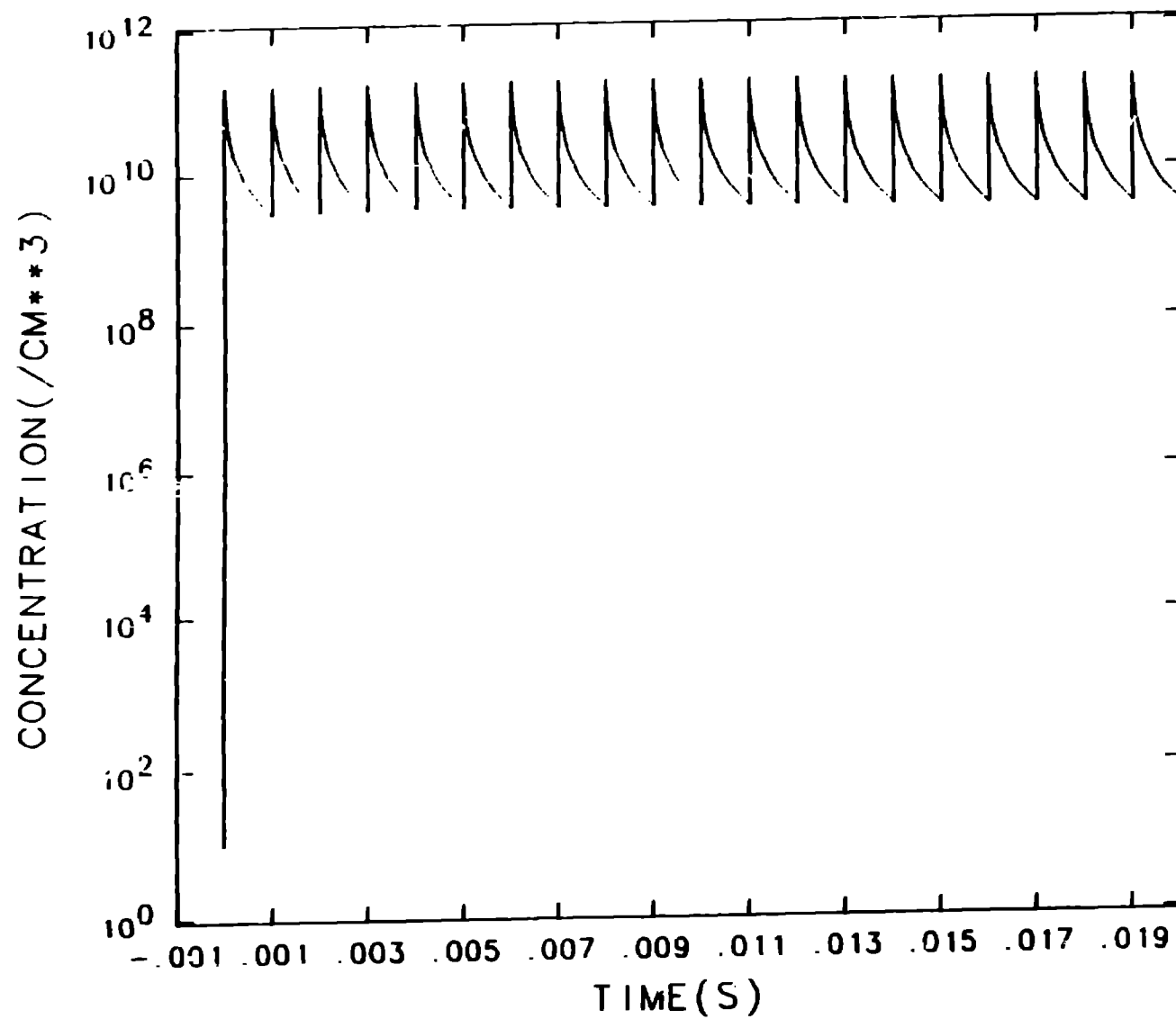
PRESSURE 1.00 (TORR)

PRESSURE 1.00 (TORR)



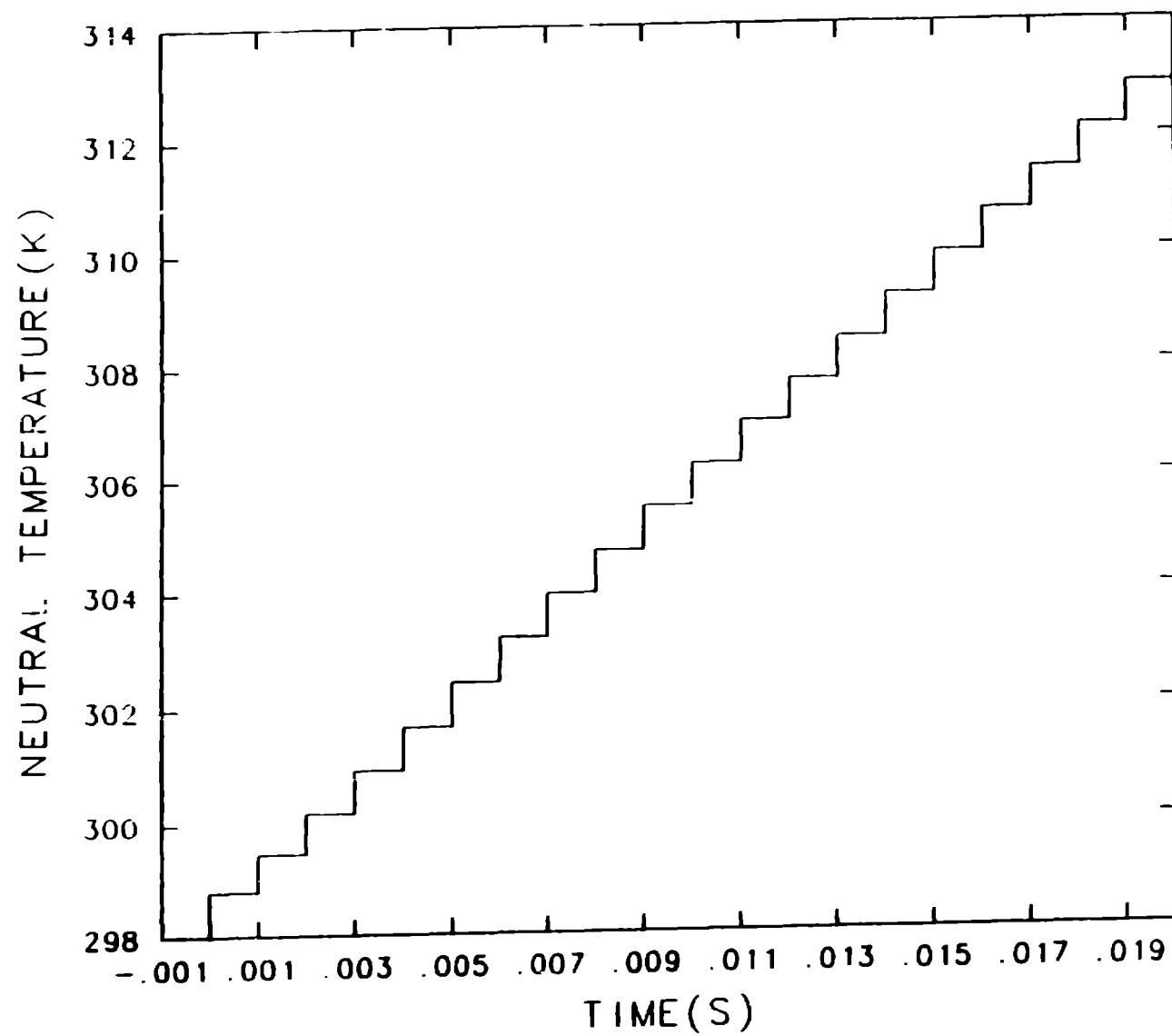
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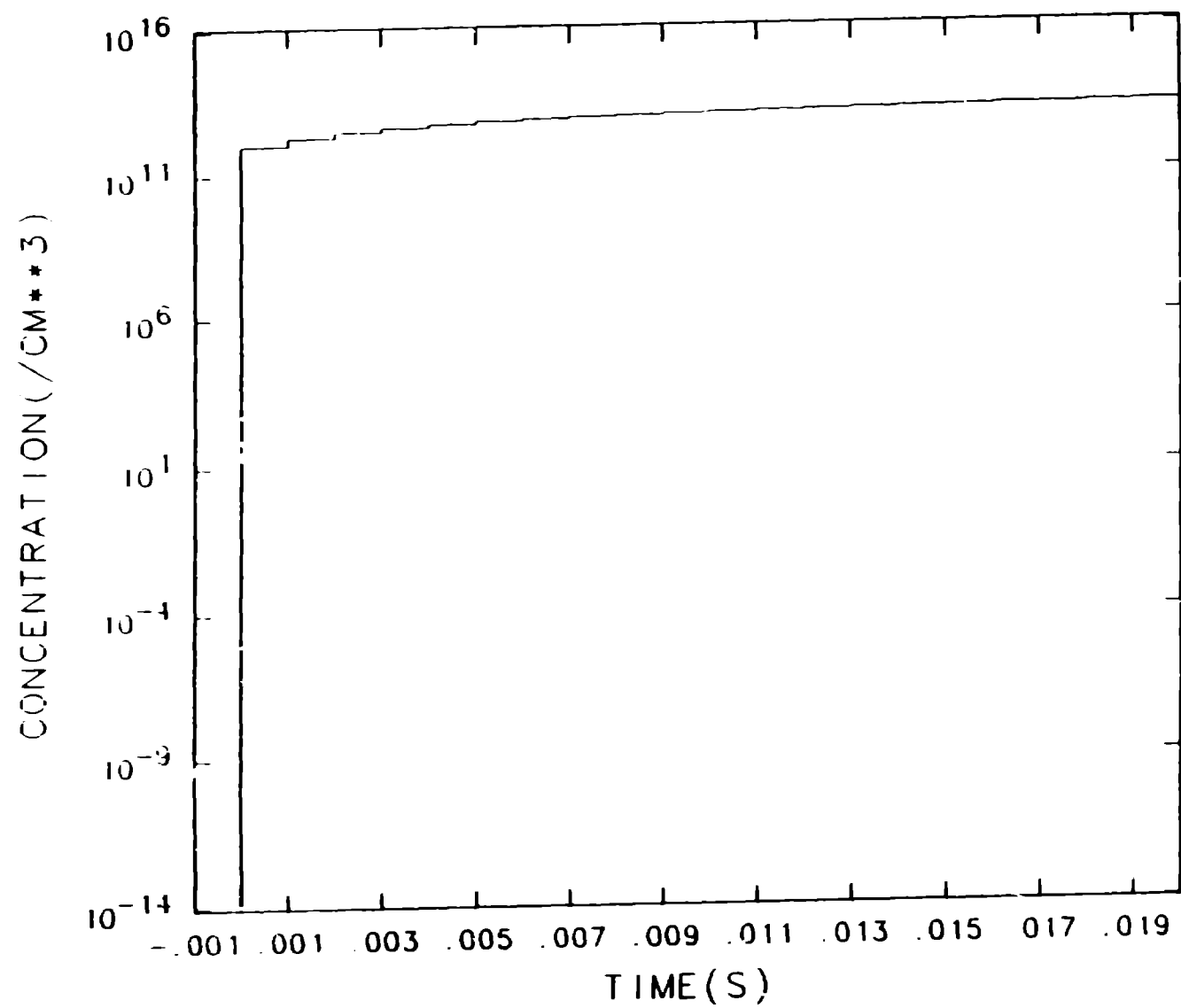


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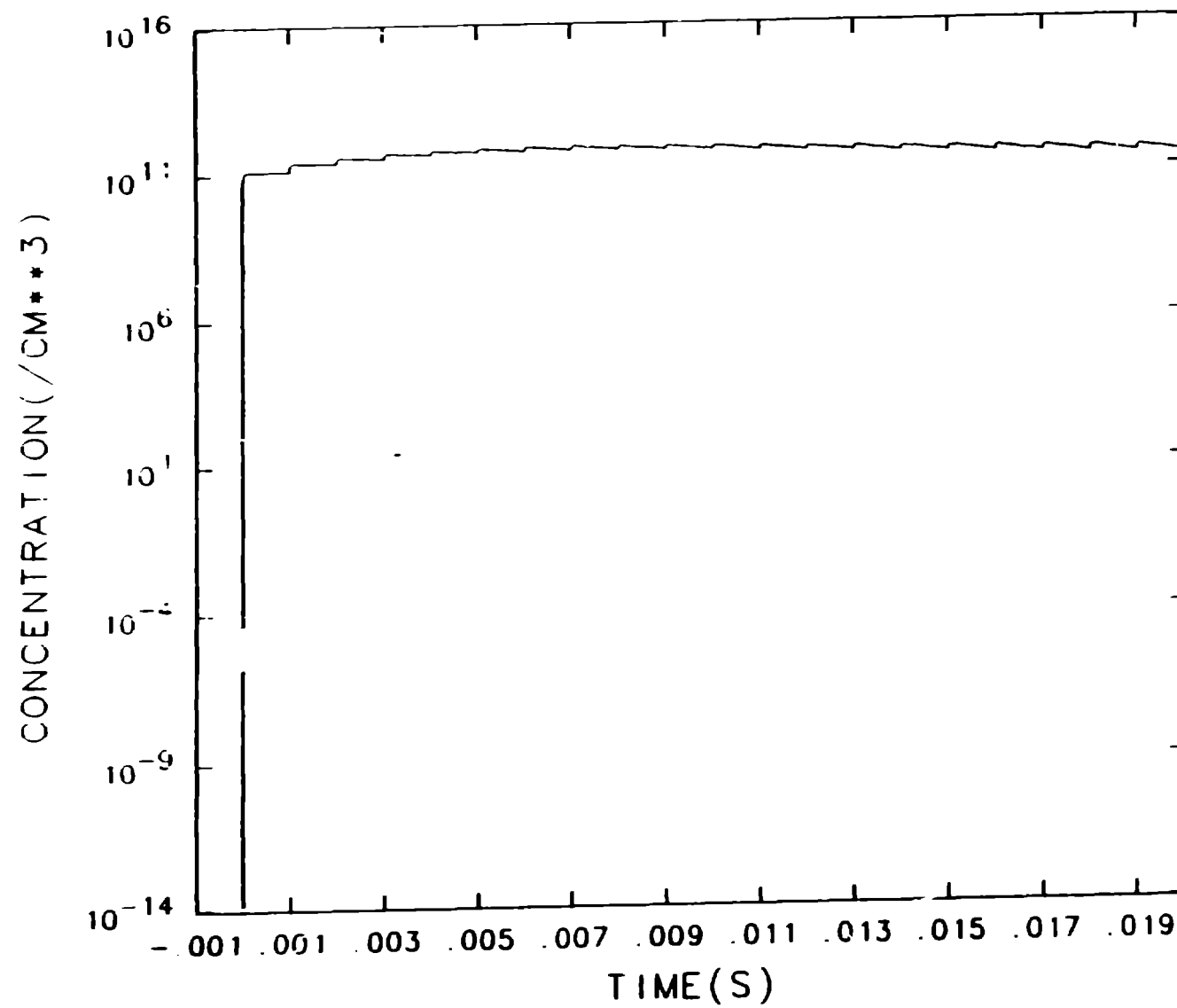
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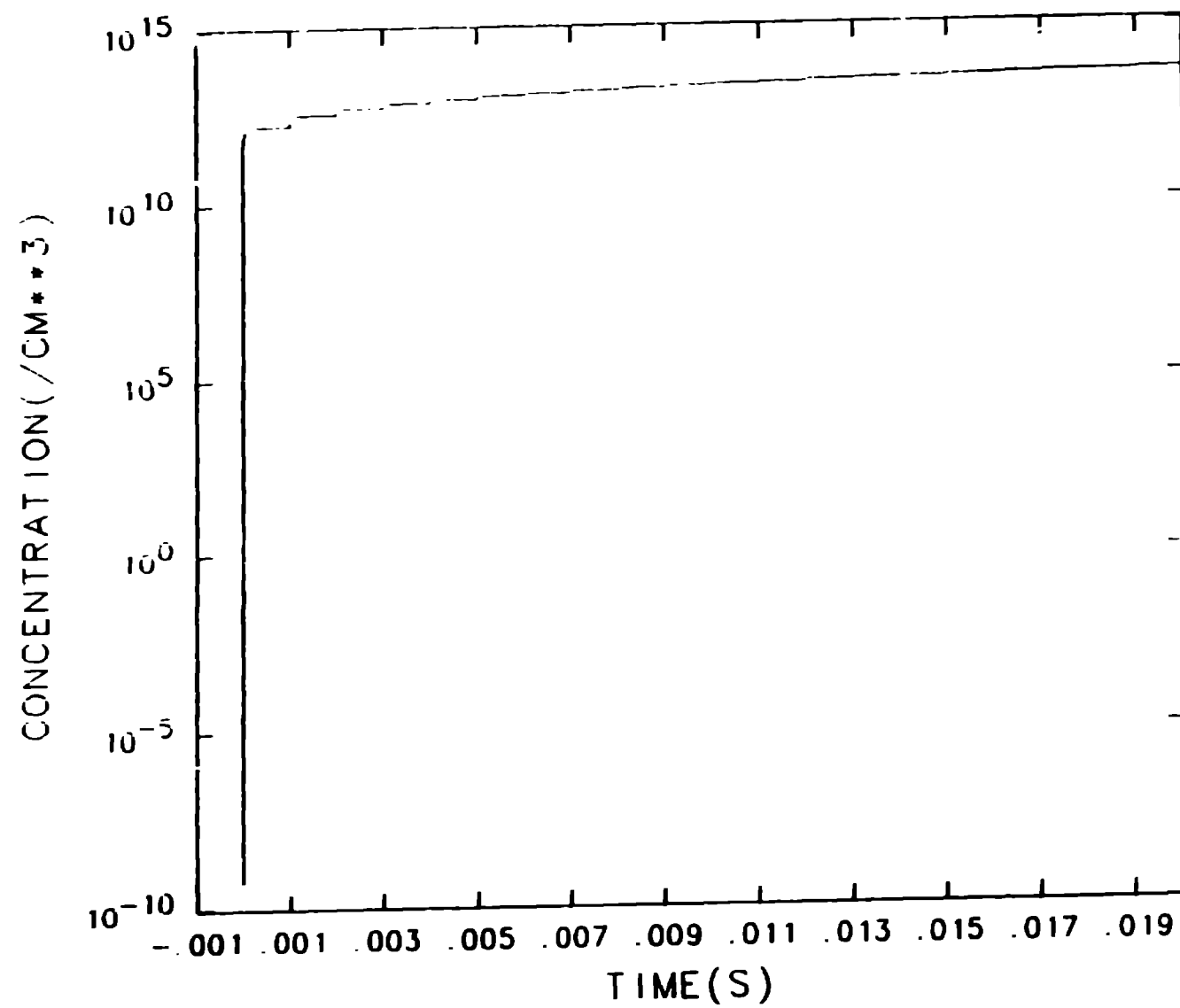
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PRESSURE 1.00 (TORR)



NO
PRESSURE 1.00 (TORR)



0
PRESSURE 1.00 (TORR)



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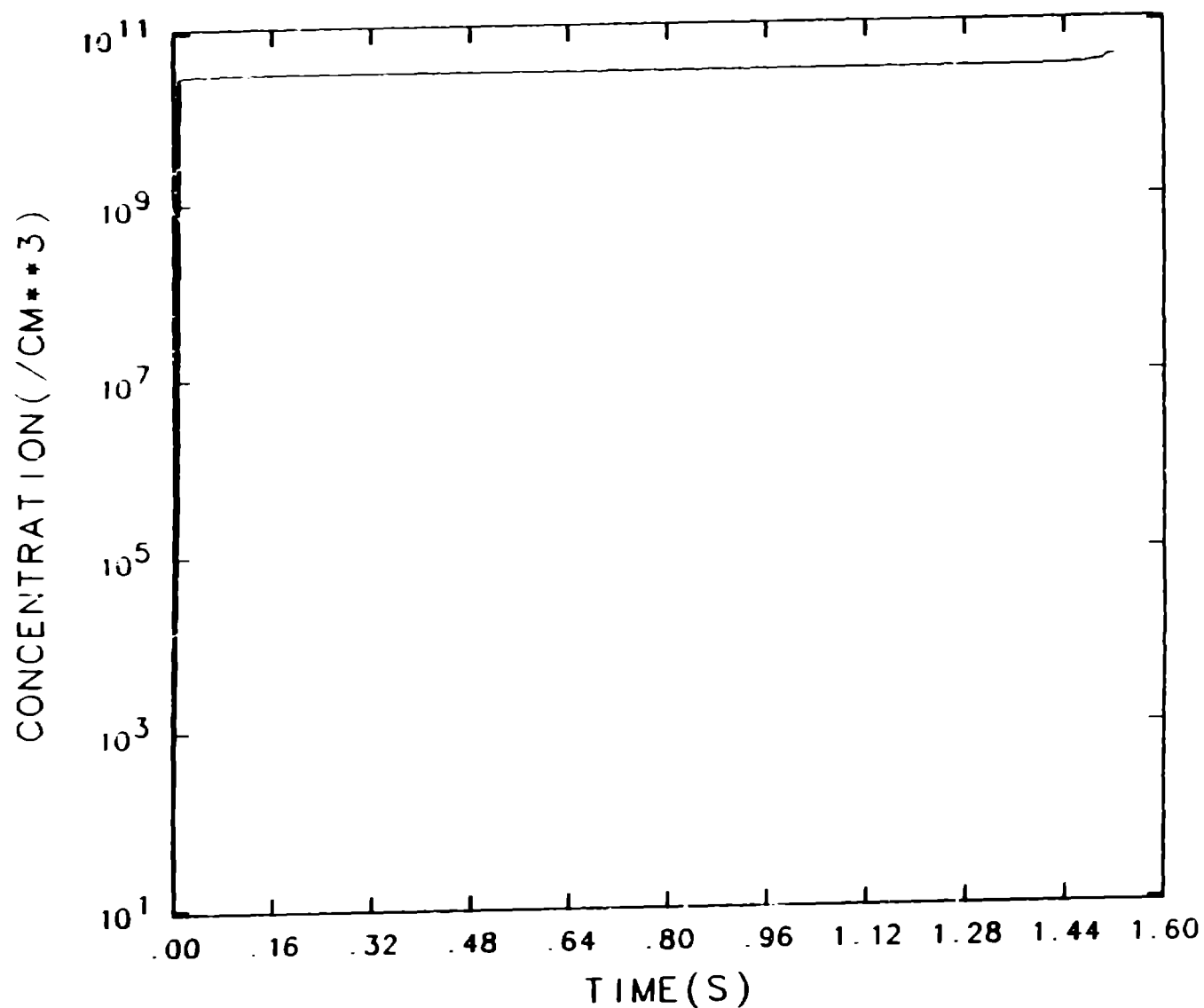
steady state

$$P = \alpha_{eff} n_e^2$$

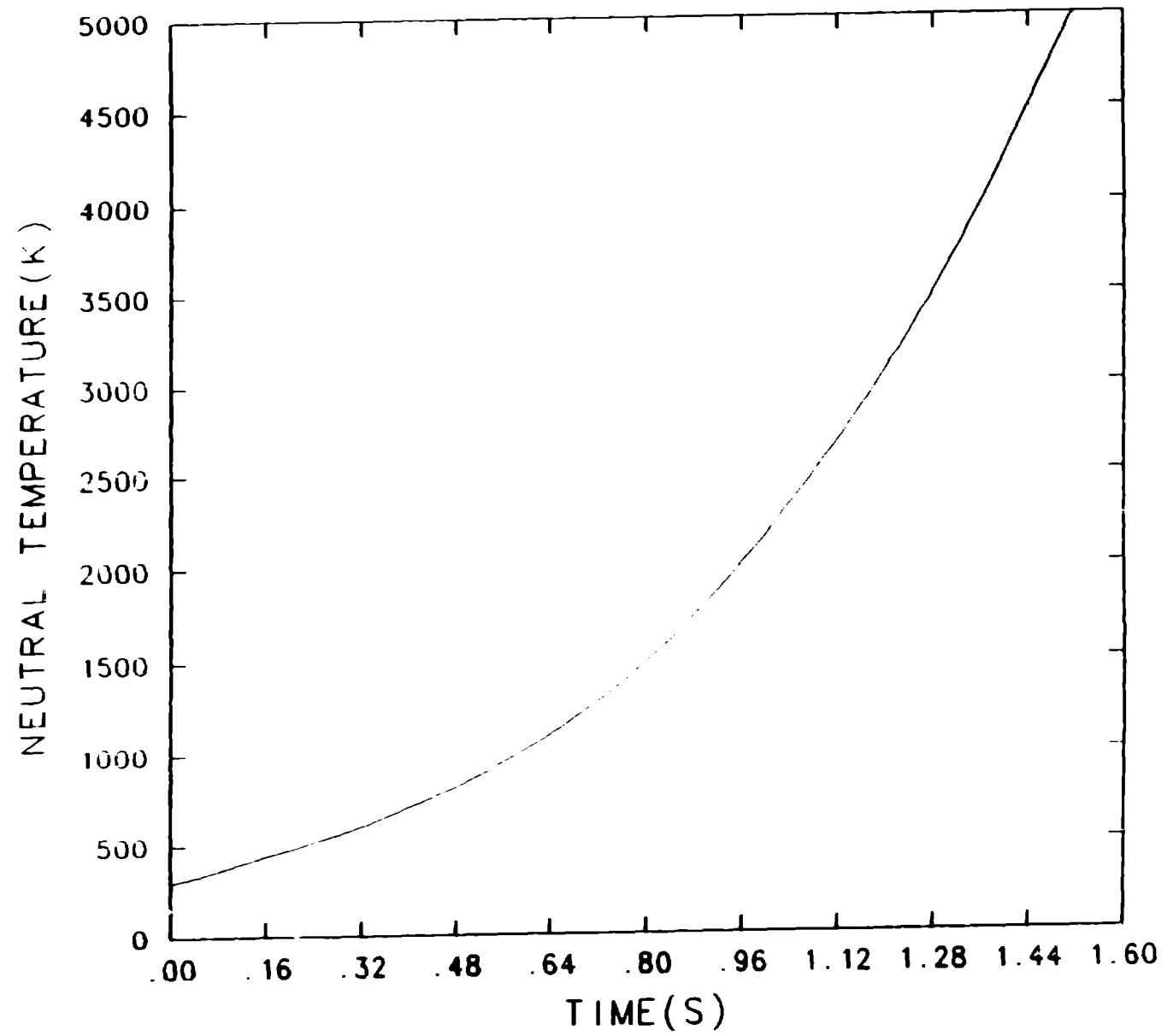
$$n_n = 3.5 \times 10^6$$

E

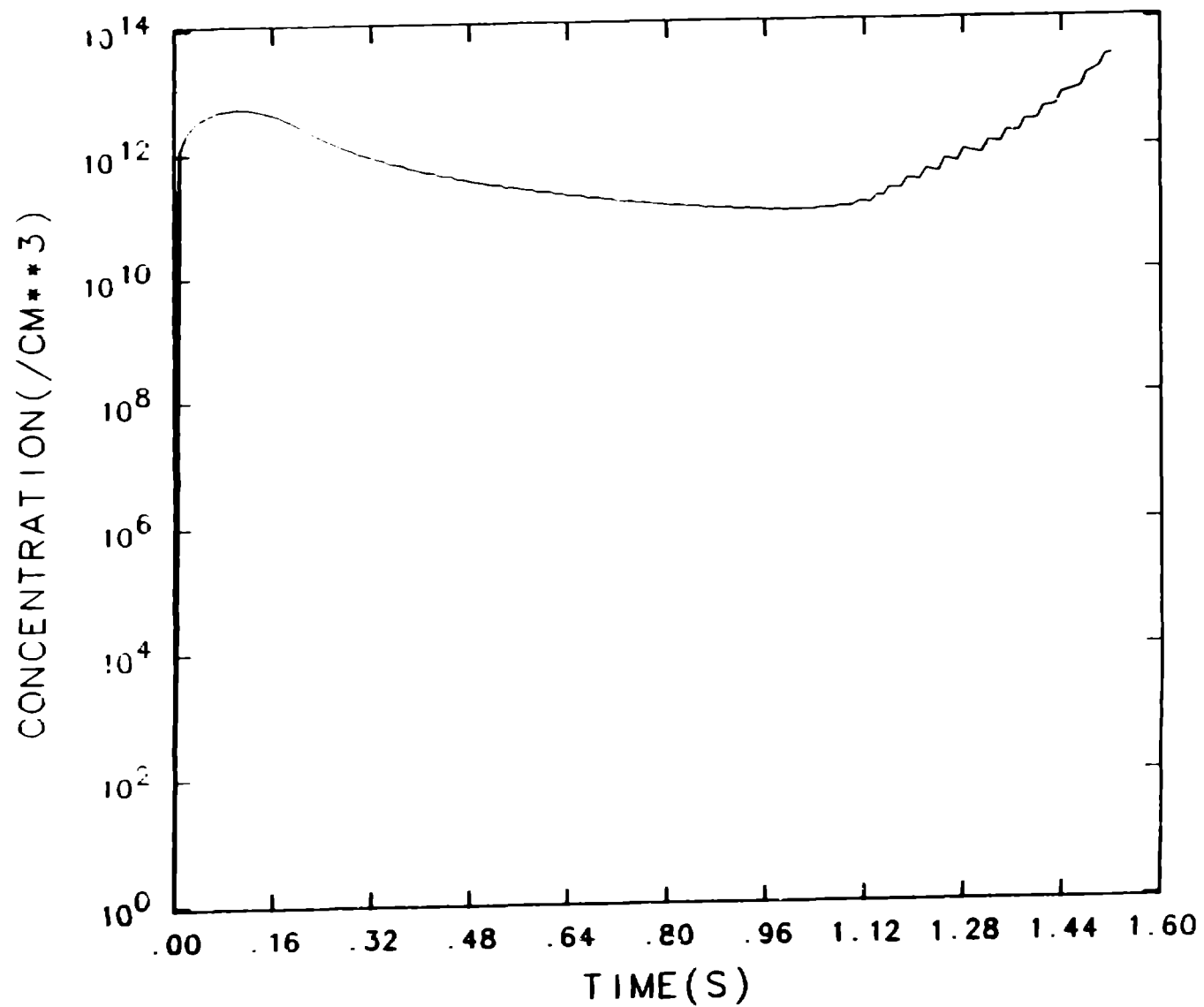
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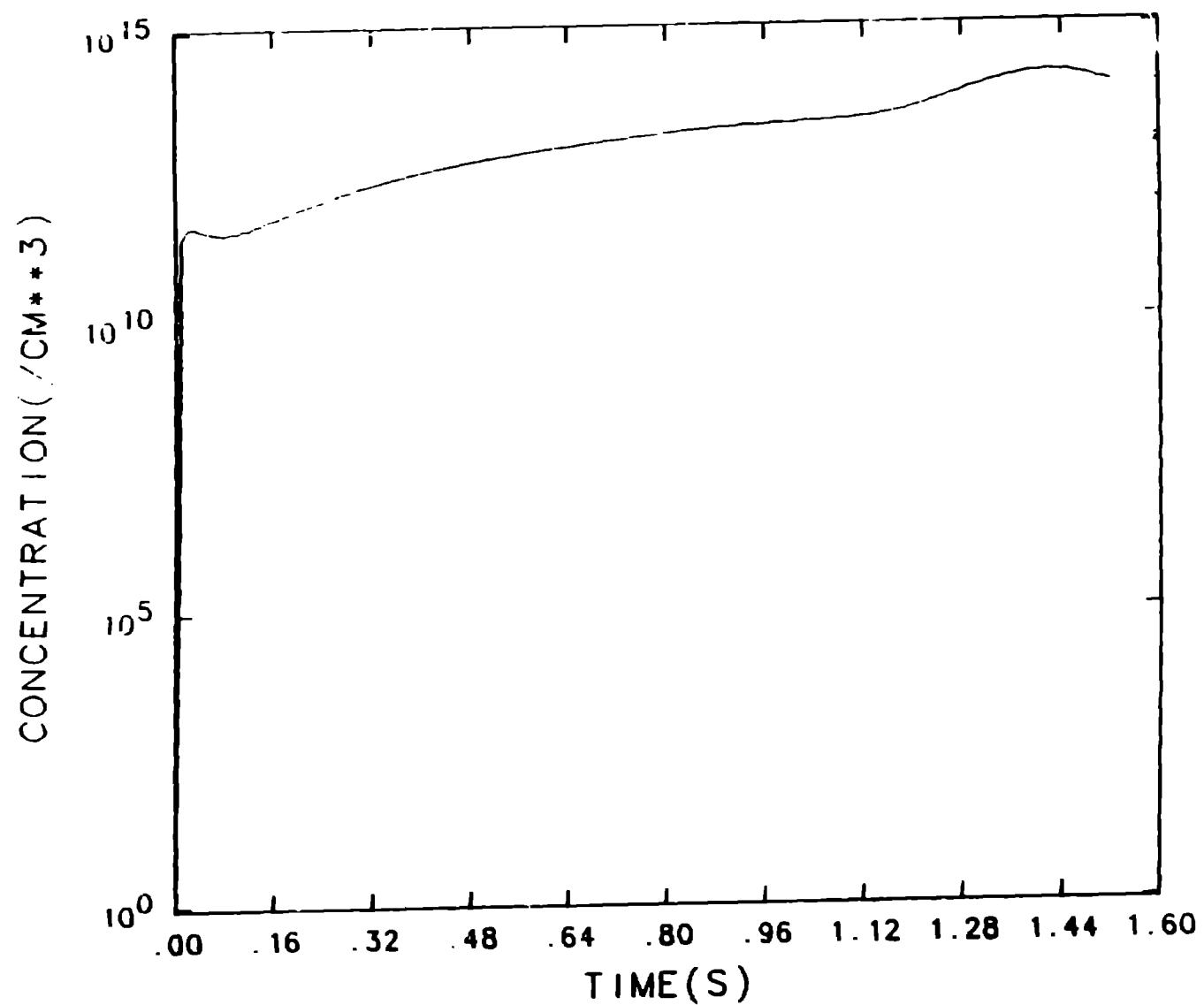
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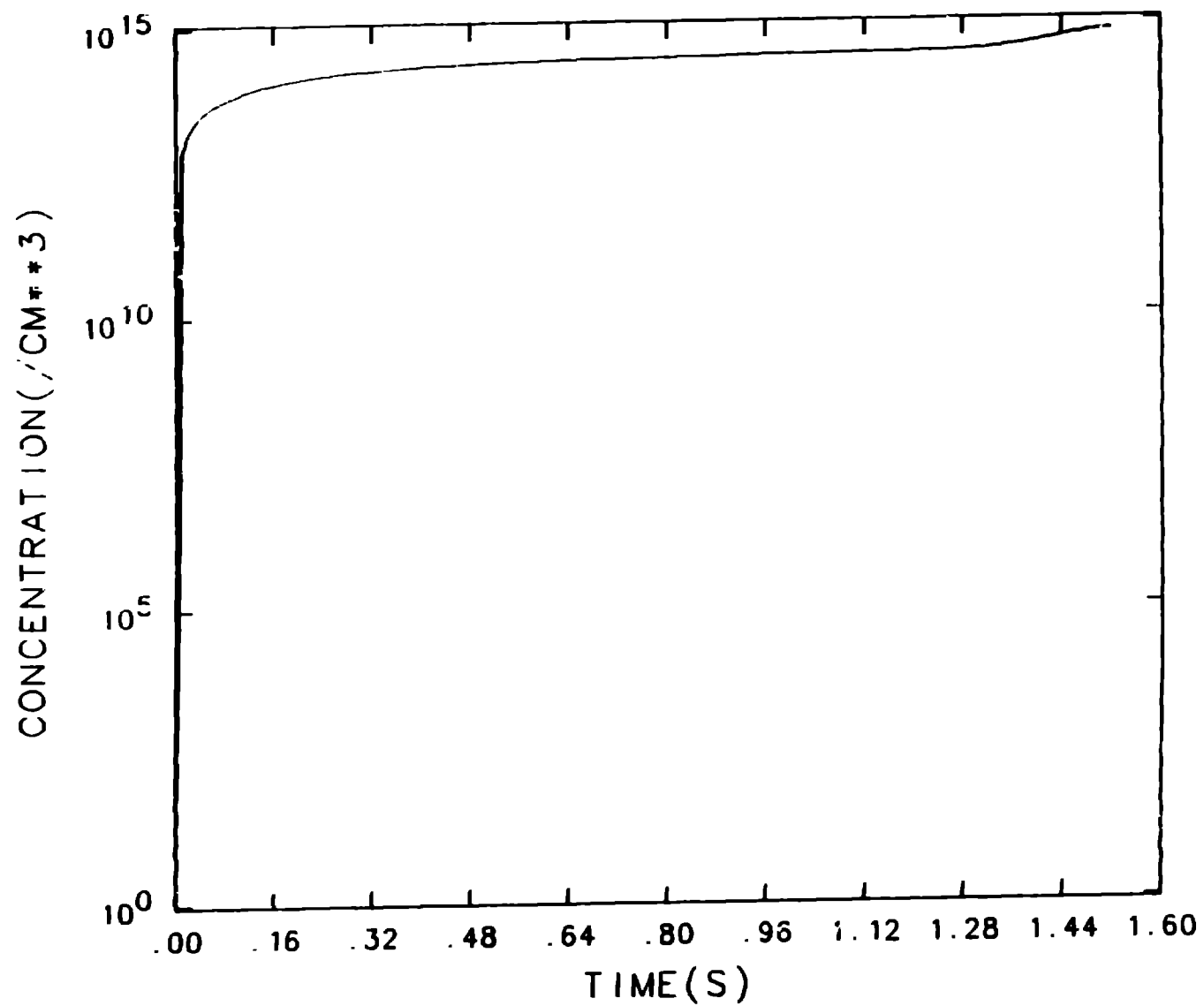
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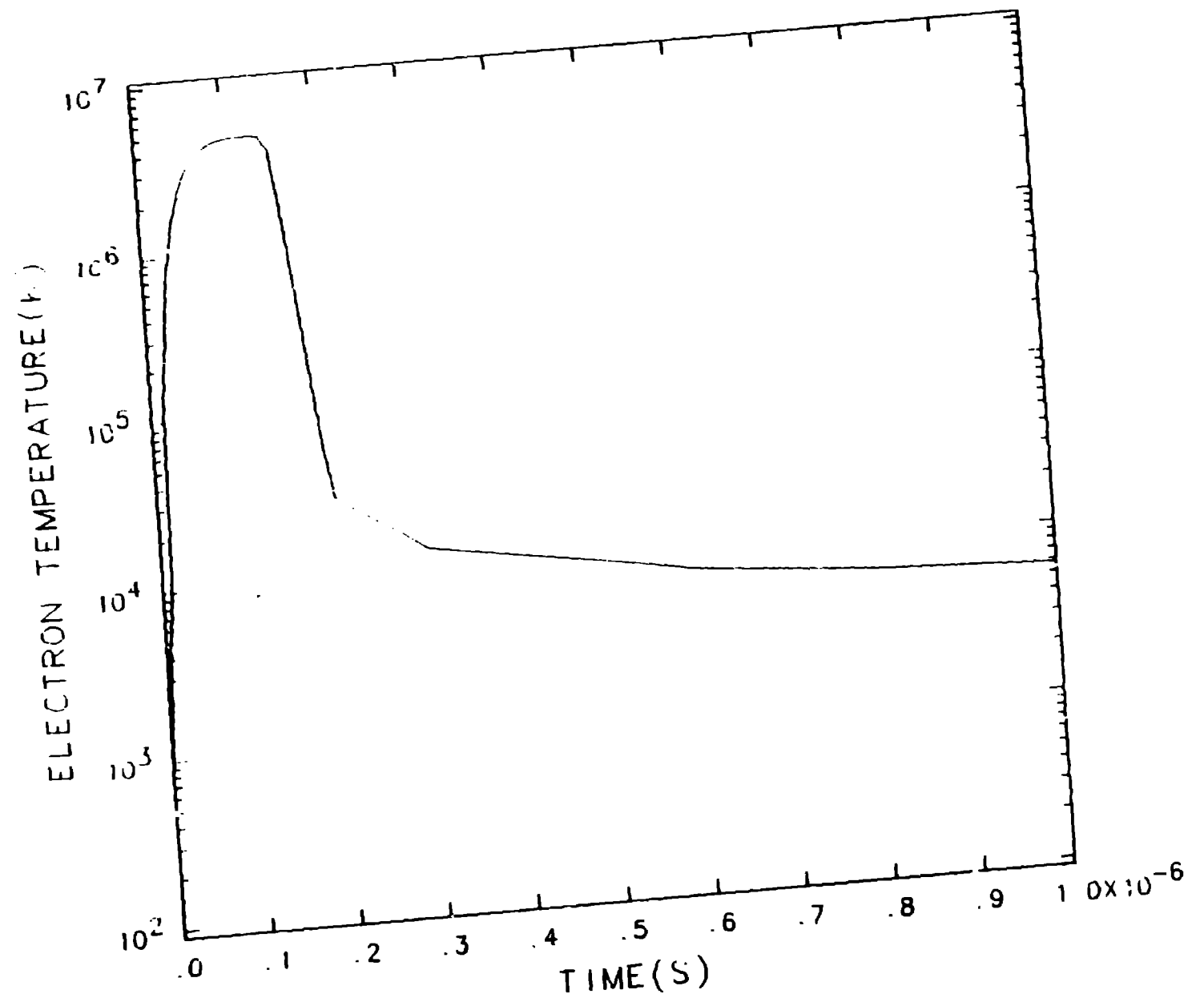
NO
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O
CONST. PRES.=1.00 TORR, NEMAX 3.40E+10

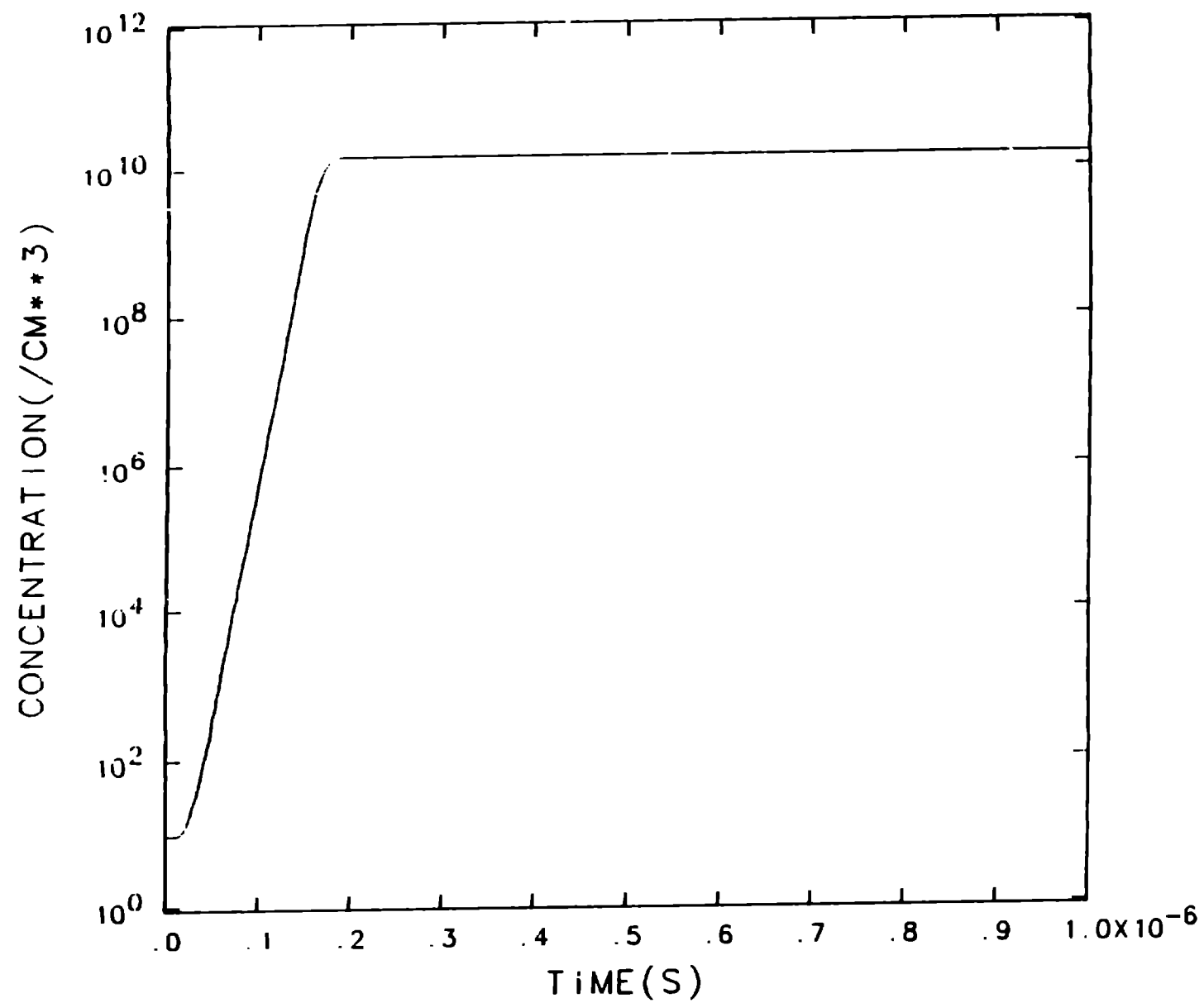


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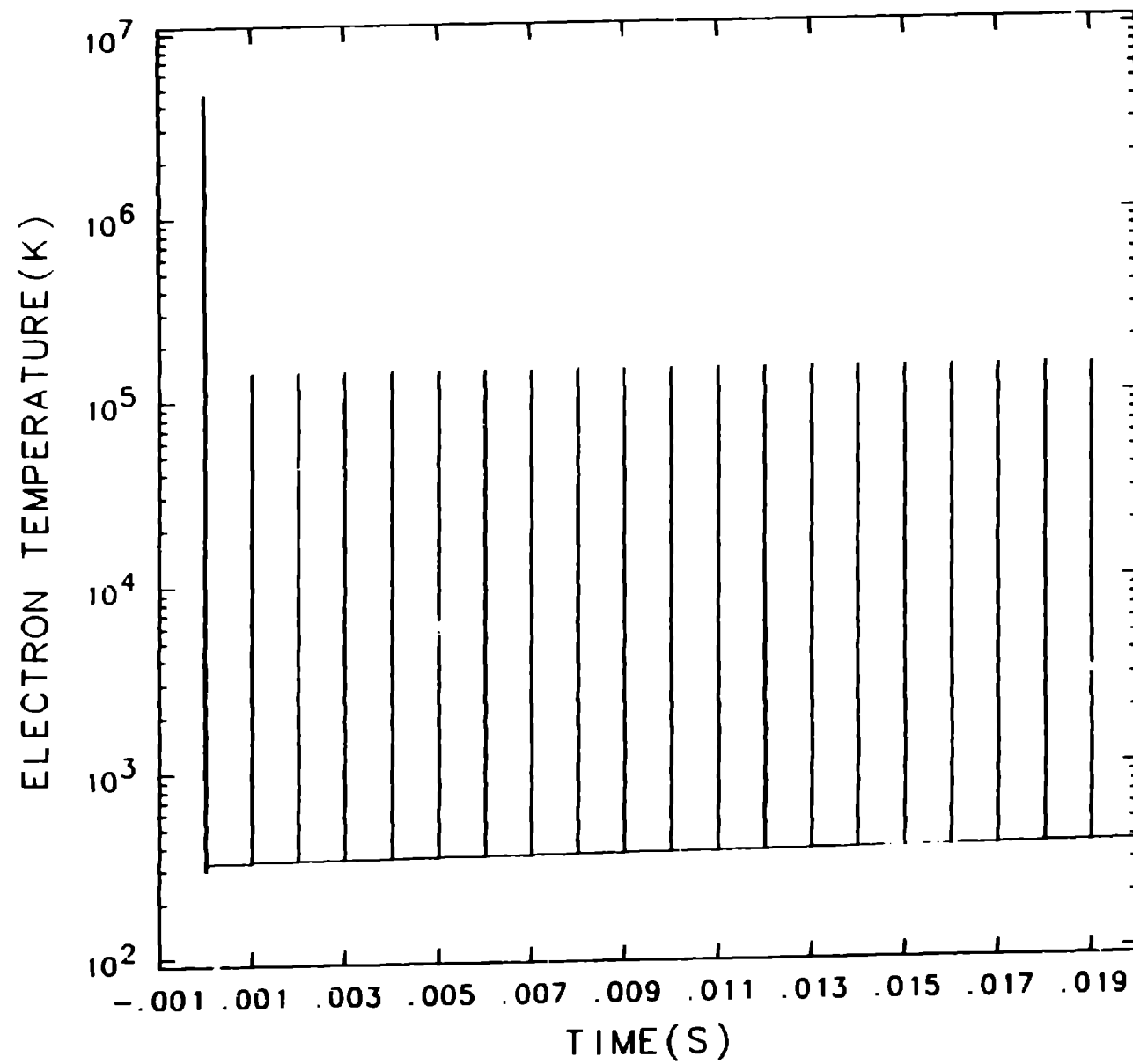


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E PRESSURE 0.03

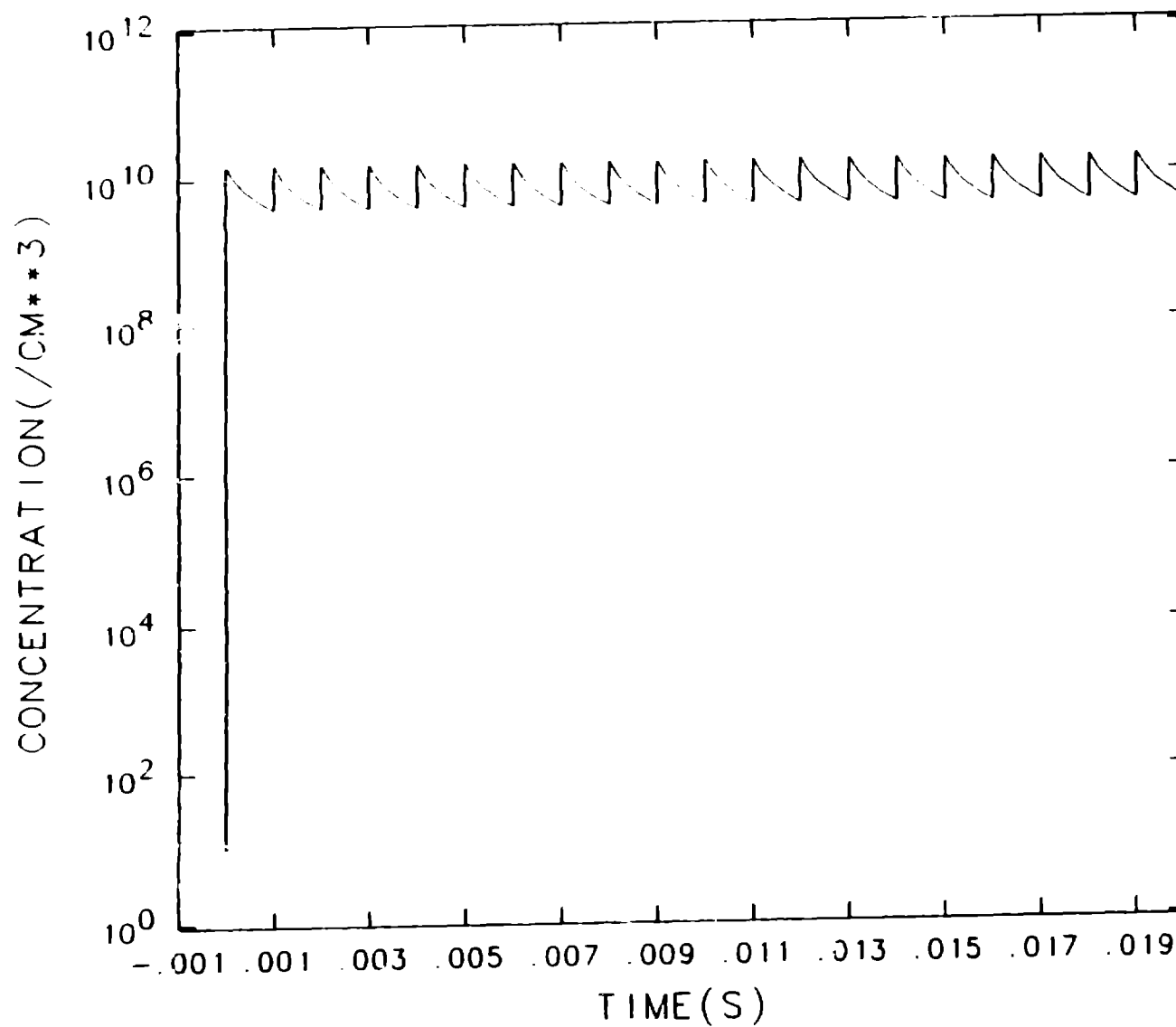


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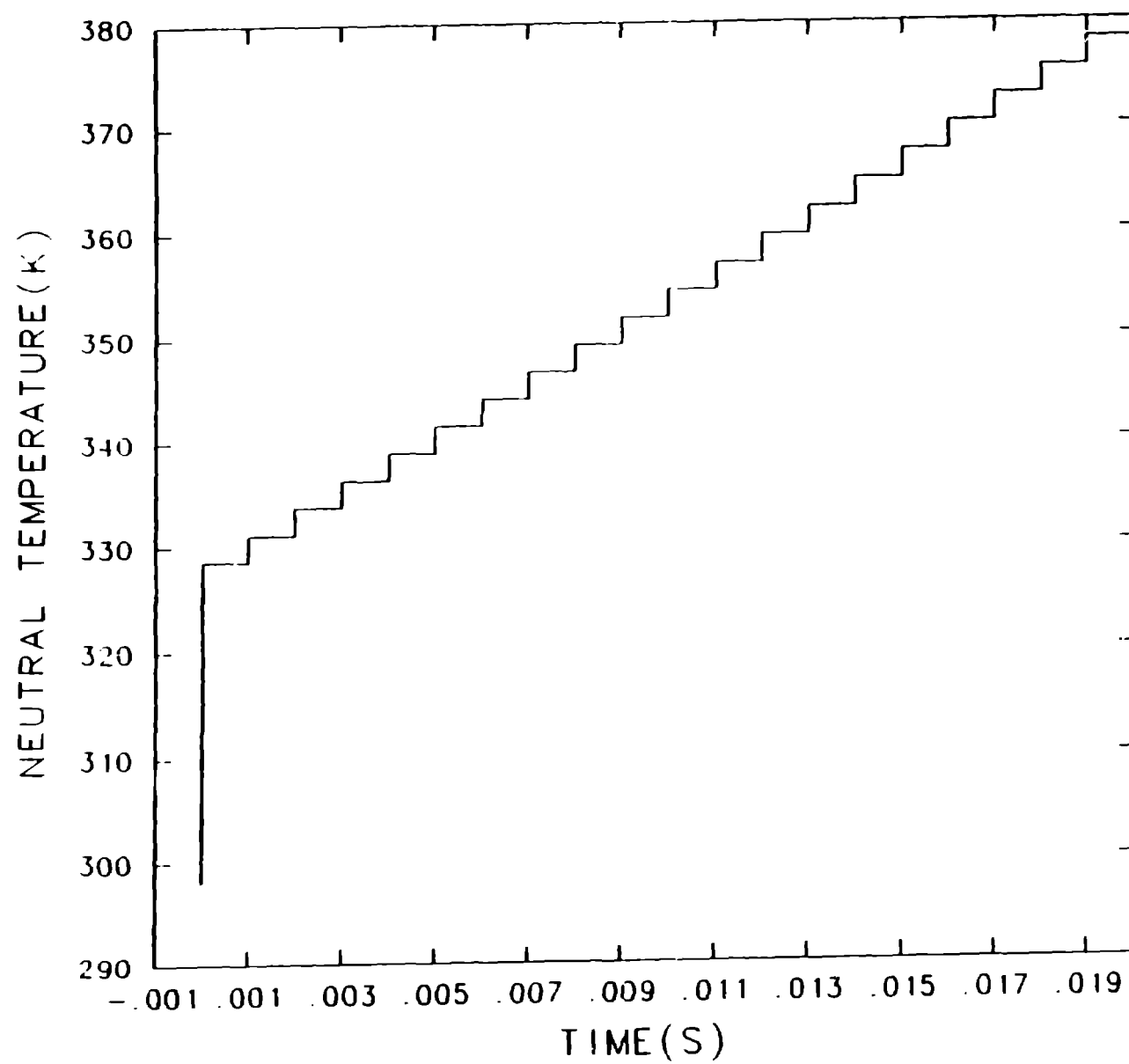


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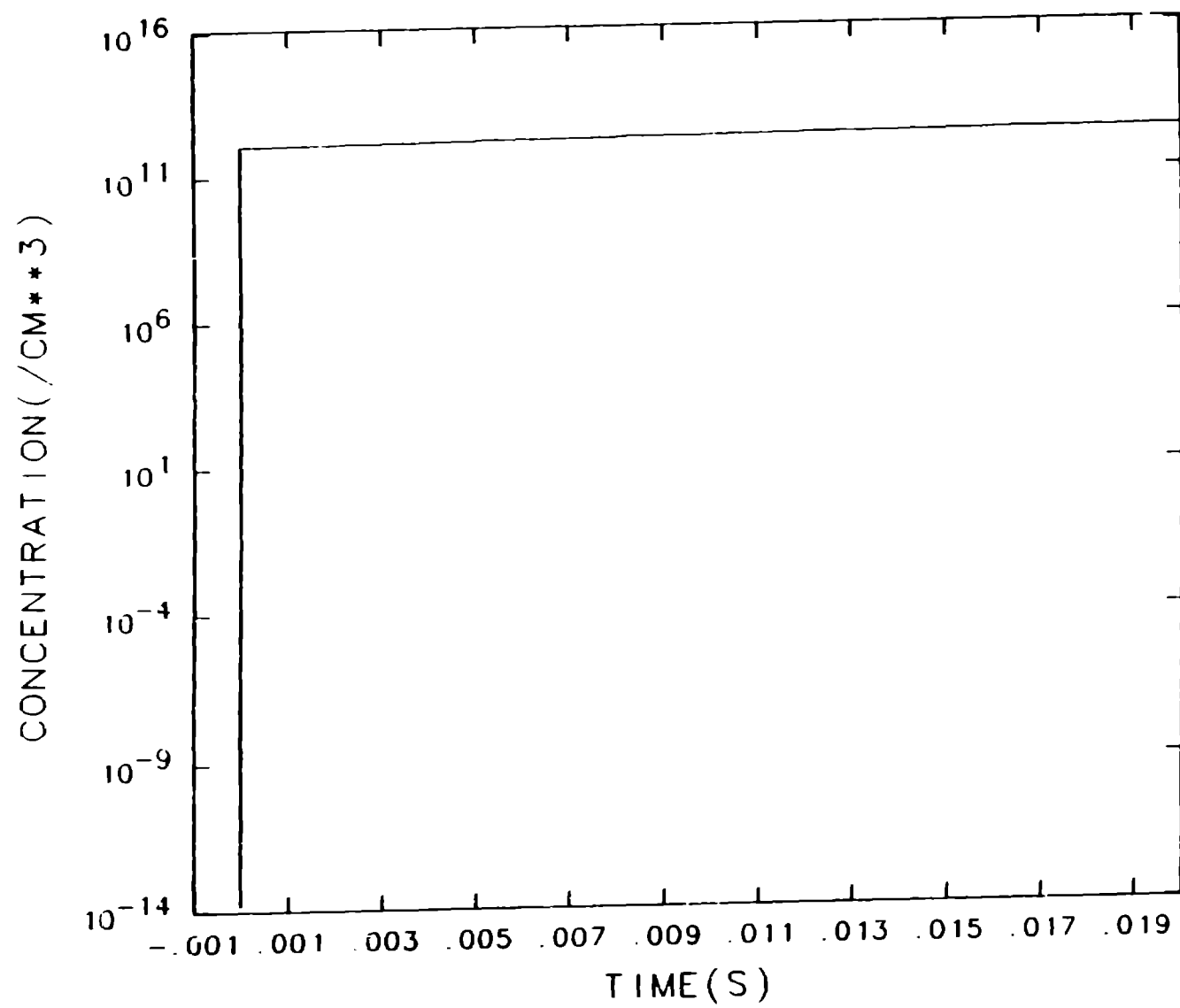
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PRESSURE 0.03 (TORR)



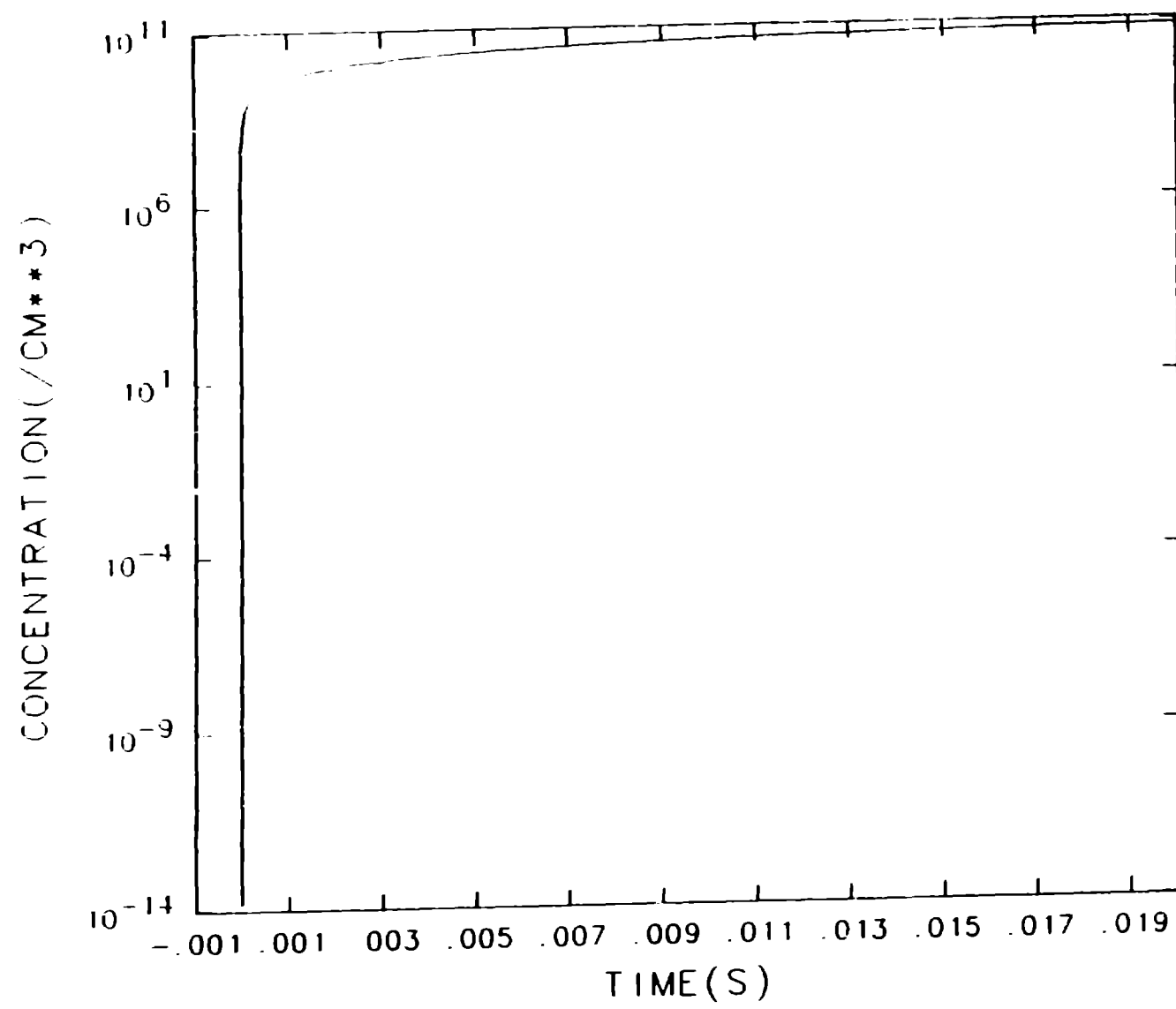
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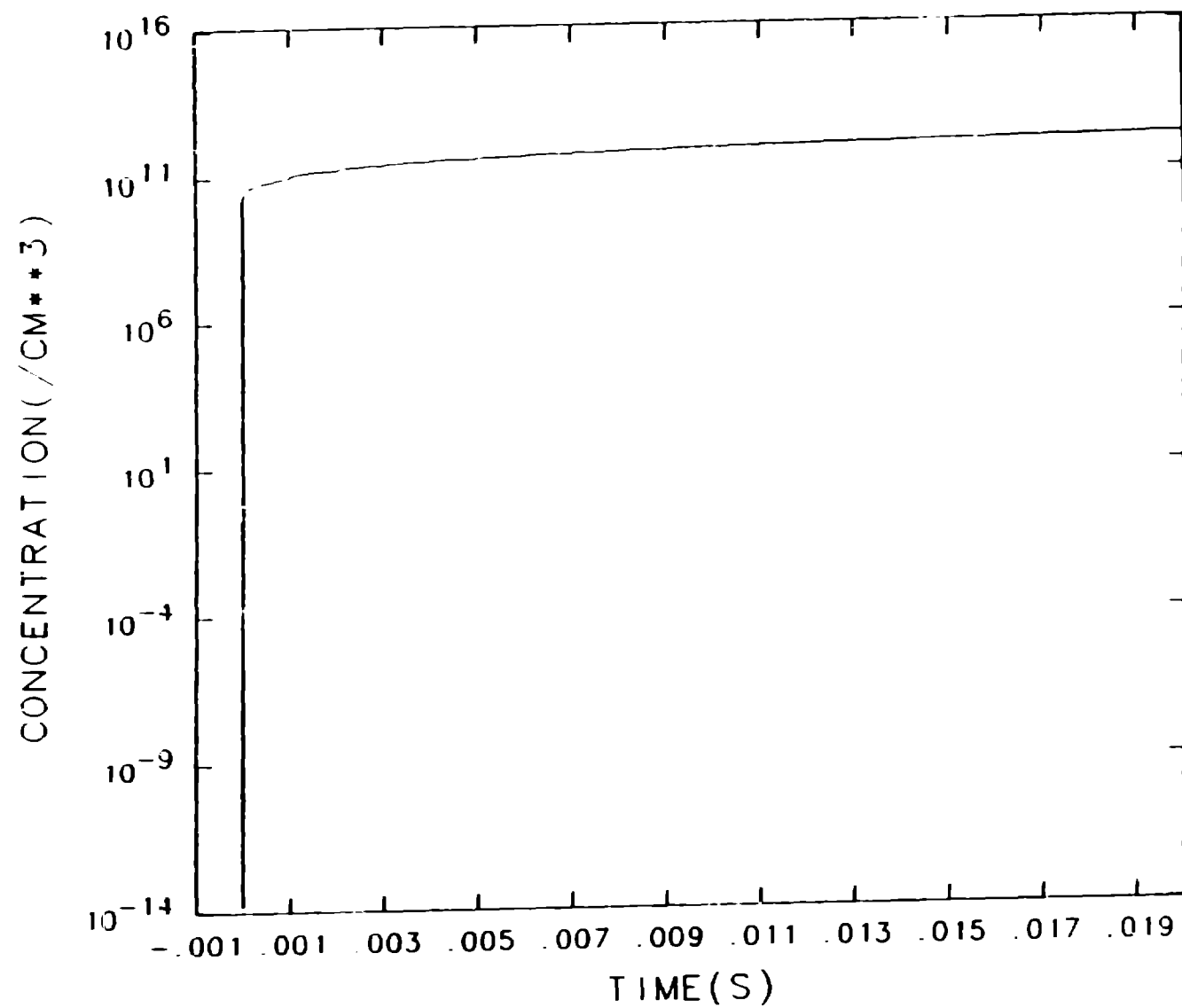
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PRESSURE 0.03 (TORR)



NO
PRESSURE 0.03 (TORR)



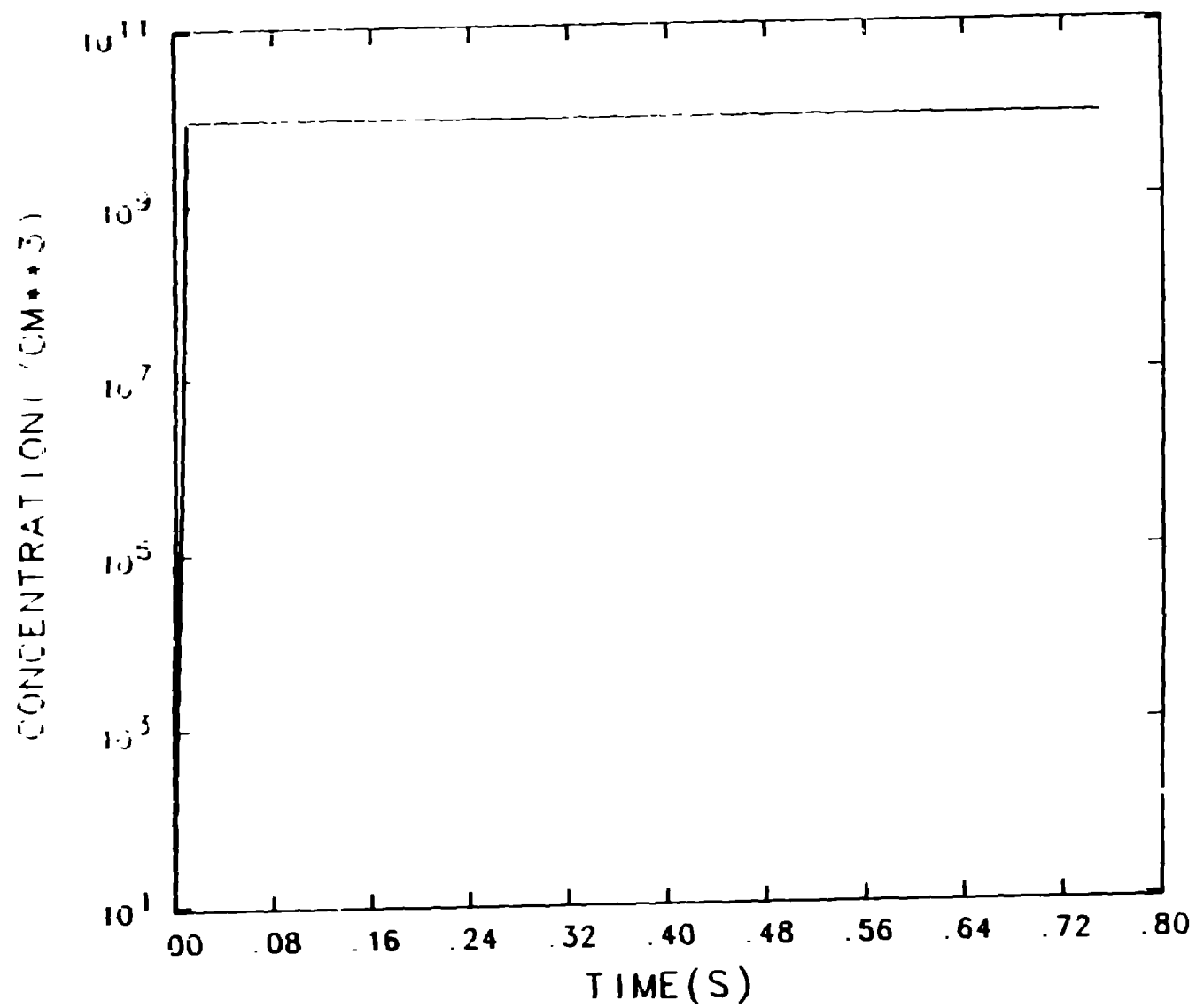
O
PRESSURE 0.03 (TORR)



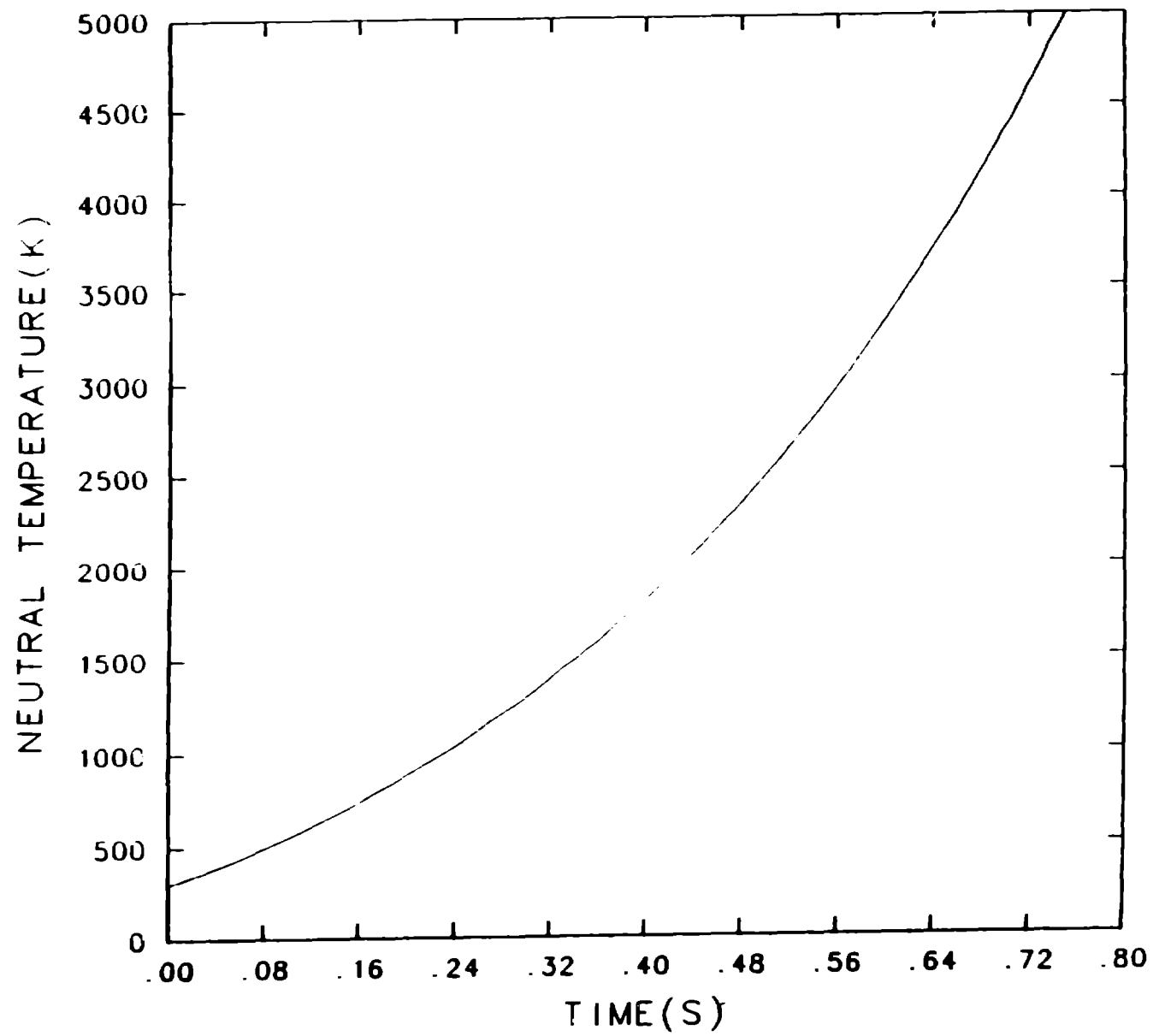
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E

CONST. PRES.=0.03 TORR, NEMAX 1.00E+10

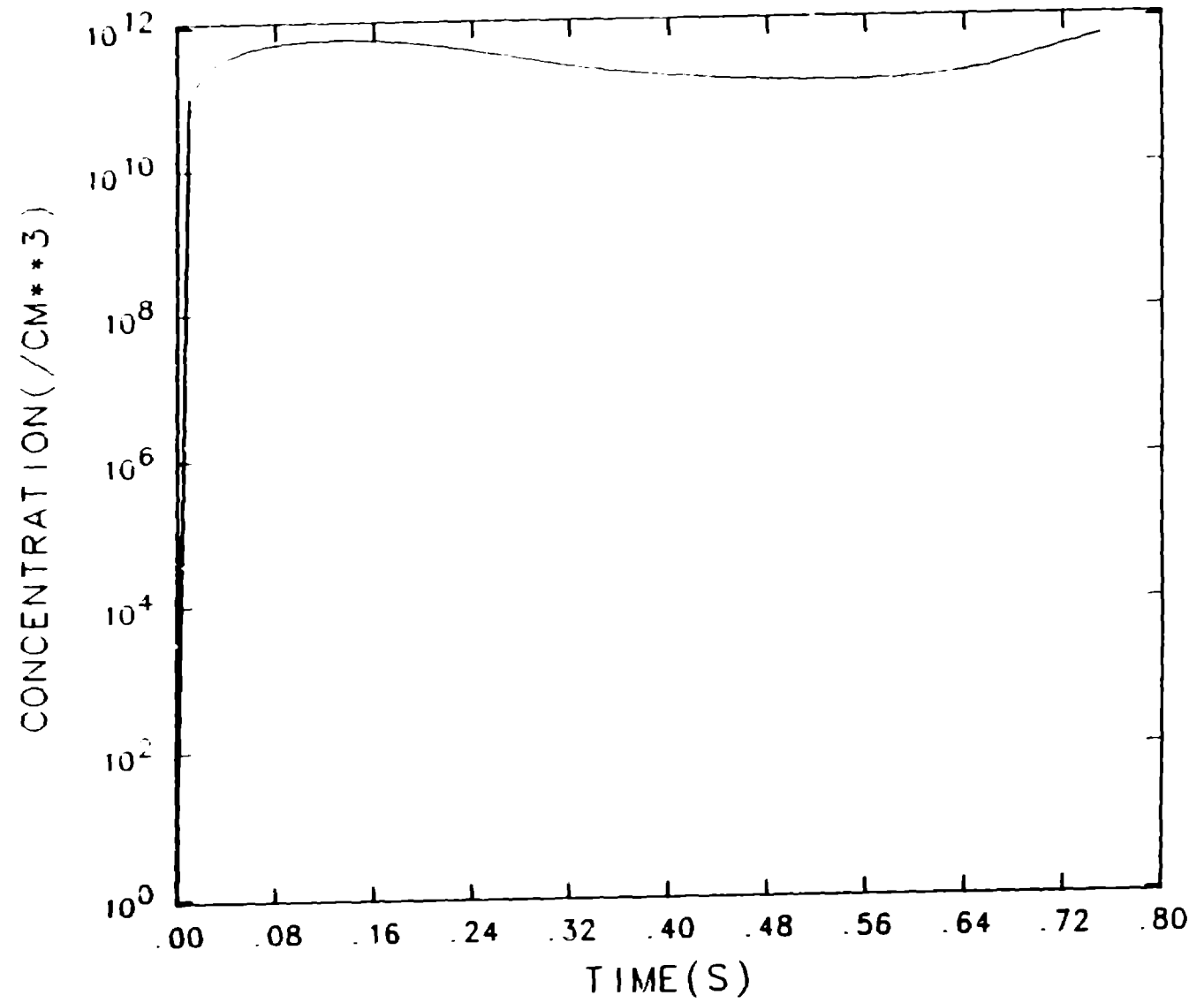


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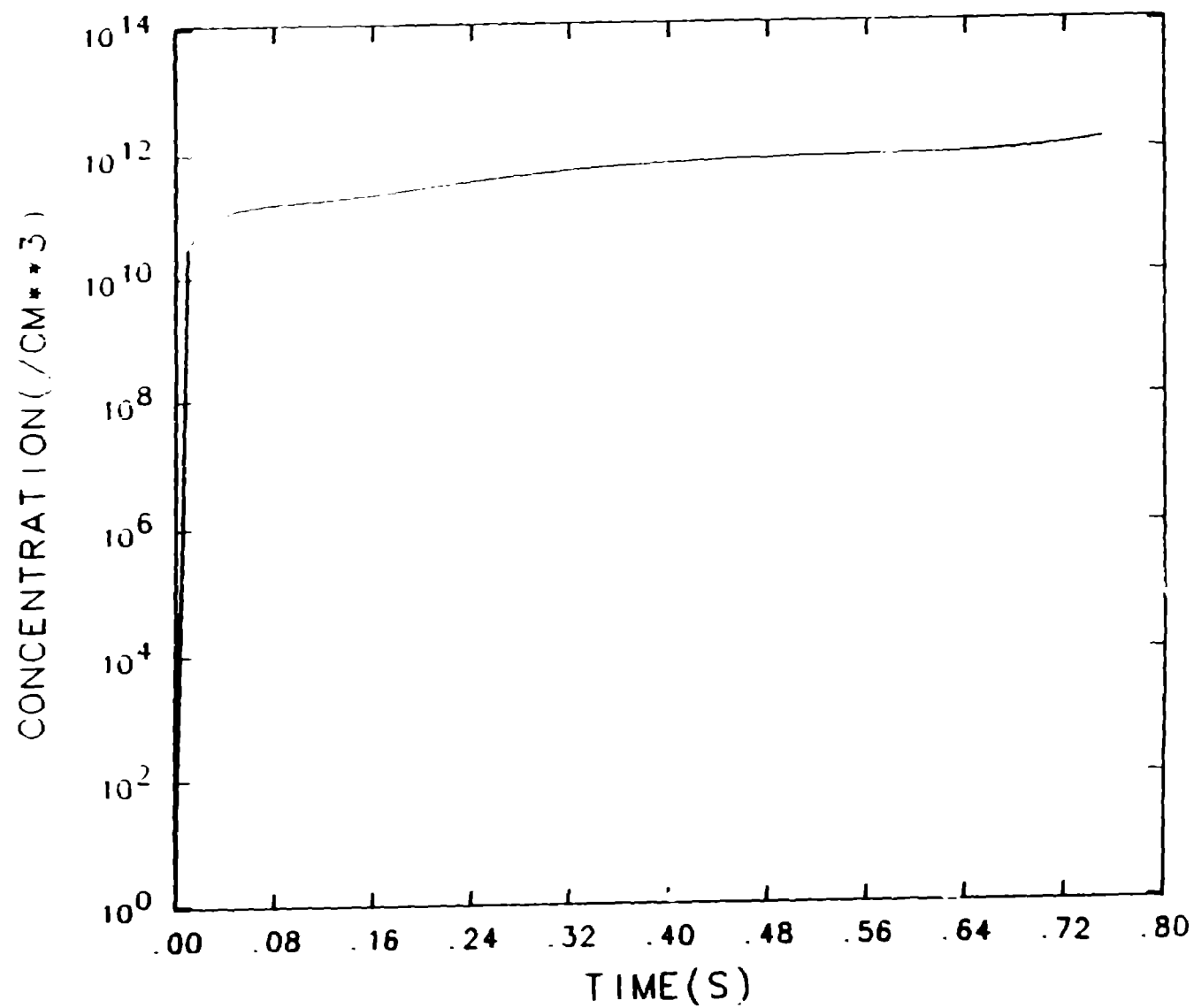


II

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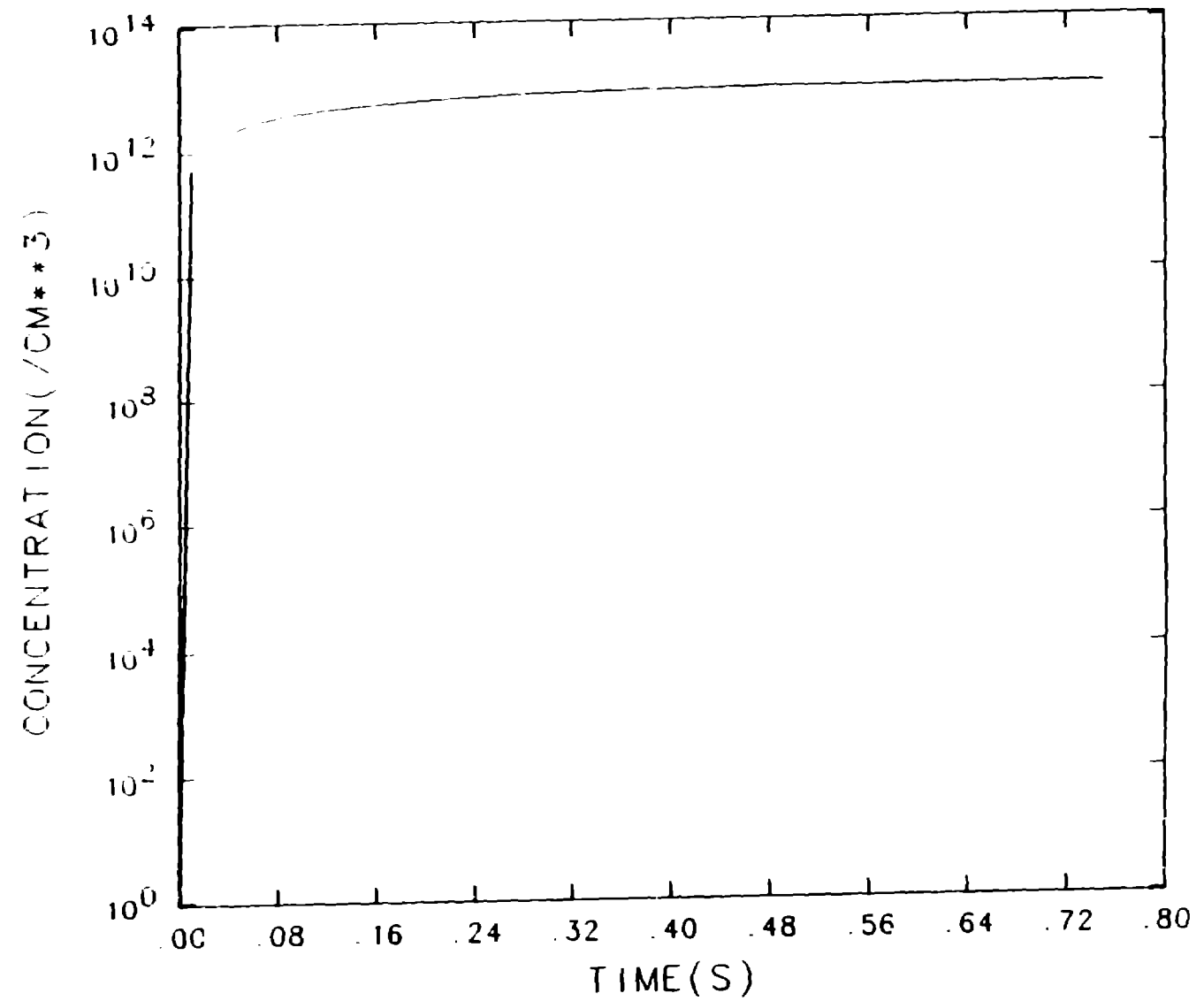


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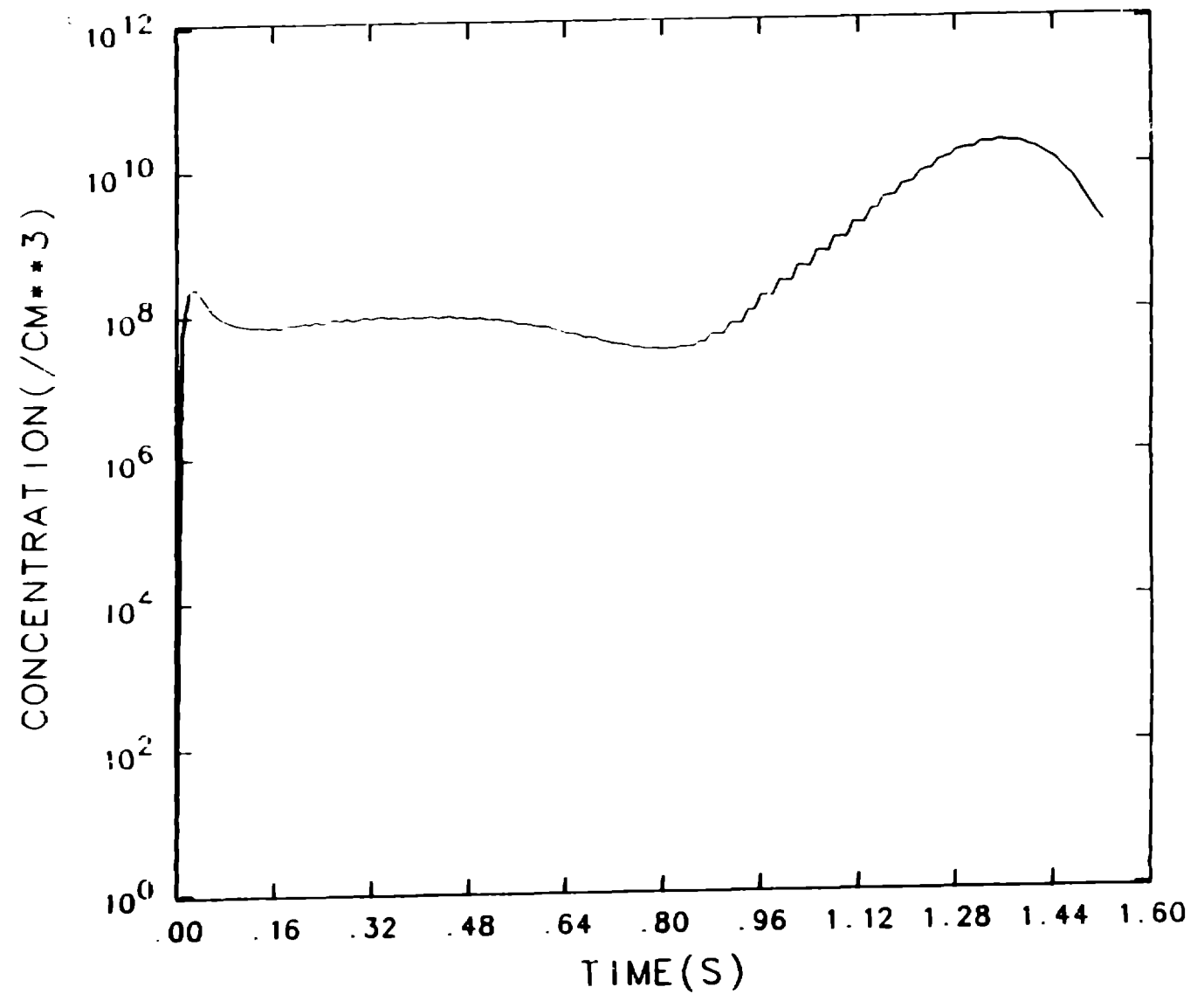
O

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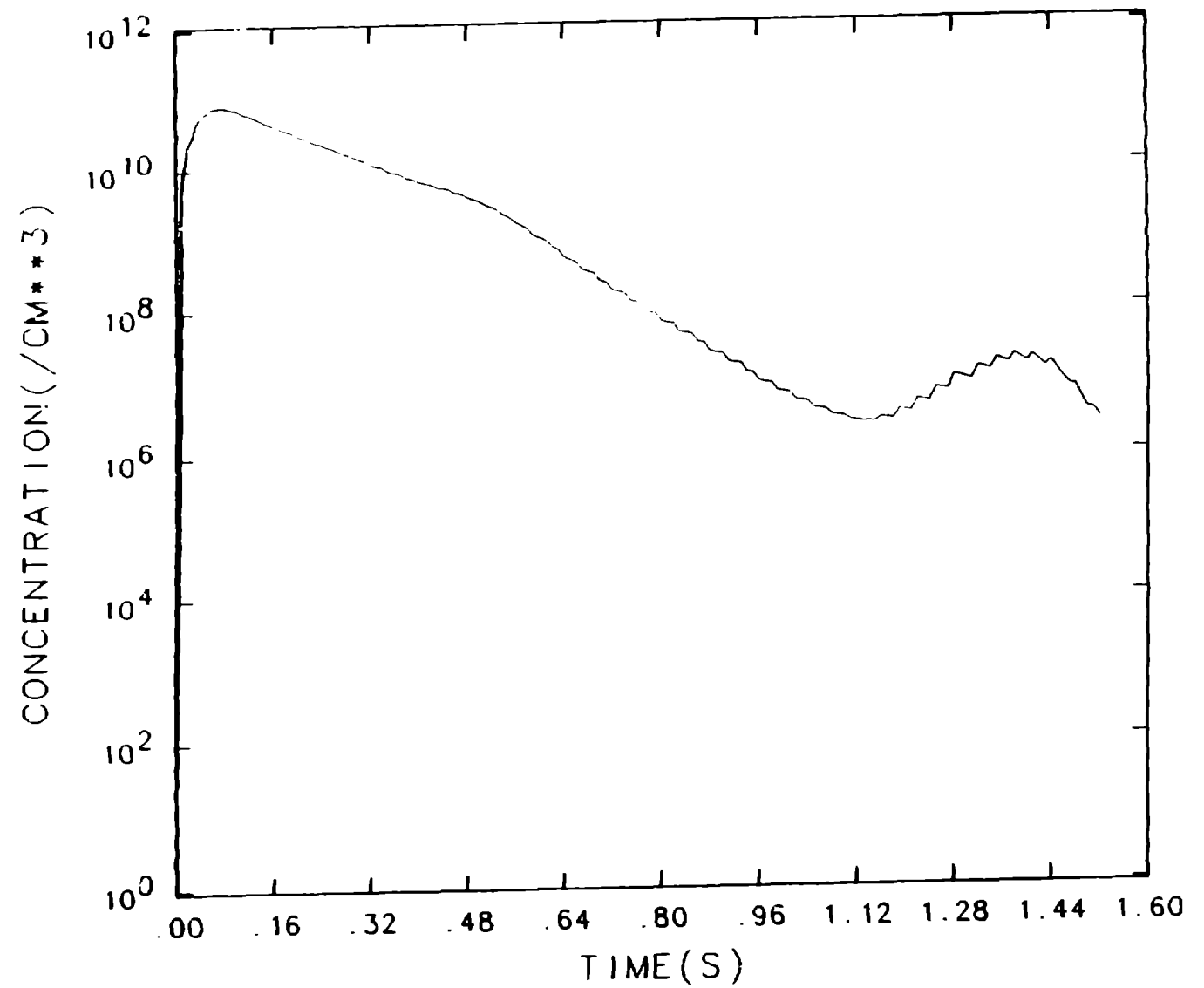
NO2

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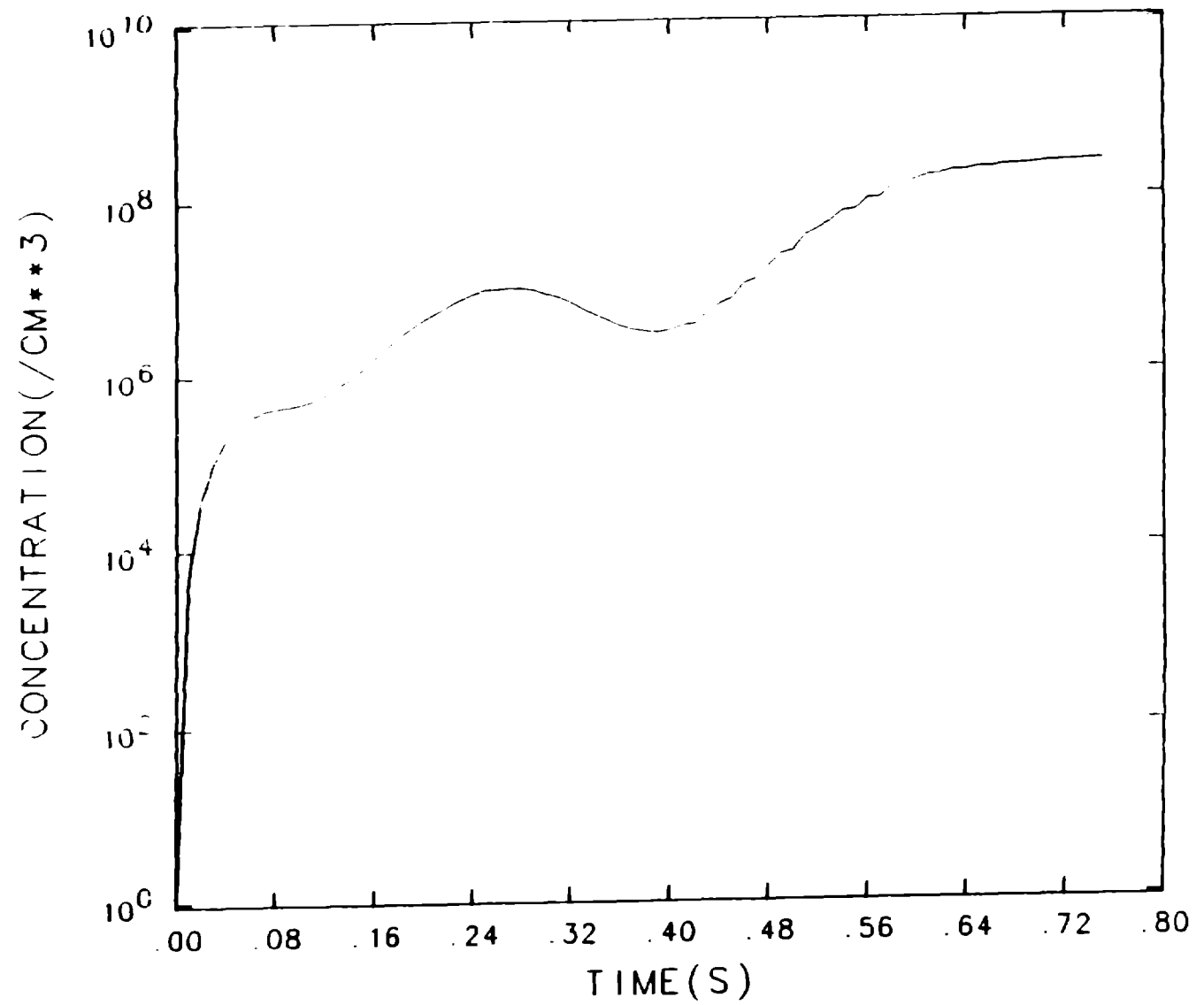
03

CONST. PRES.=1.00 TORR, NEMAX 3.40E+10



NO2

CONST. PRES.=0.03 TORR, NEMAX 1.00E+10



O3
CONST. PRES.=0.03 TORR, NEMAX 1.00E+10

